A new approach for electronic heat conduction in molecular dynamics simulations

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Abstract
We present a new approach for the two-temperature molecular dynamics (MD) model for coupled simulations of electronic and phonon heat conduction in nanoscale systems. The proposed method uses a master equation to perform heat conduction of the electronic temperature eschewing the need to use a basis set to evaluate operators. This characteristic allows us to seamlessly couple the electronic heat conduction model with MD codes without the need to introduce an auxiliary mesh. We implemented the methodology in the large-scale atomic/molecular massively parallel simulator code, and through multiple examples, we validated the methodology. We then study the effect of electron–phonon interaction in high energy irradiation simulations and the effect of laser pulse on metallic materials. We show that the model provides an atomic level description in complex geometries of energy transfer between electrons and phonons. Thus, the proposed approach provides an alternative way to the two-temperature MD models. The parallel performance and some aspects of the implementation are presented.

Keywords: nanoscale heat transport, electronic heat conduction, two-temperature model, kinematic mean field theory, irradiation damage, laser ablation

(Some figures may appear in colour only in the online journal)

1. Introduction

Classical molecular dynamics (MD) simulations have been used widely in materials physics to study the lattice and defect dynamics at the atomic scale in both equilibrium and
non-equilibrium conditions. In classical MD, the thermal conductivity due to lattice contribution is considered, since the phonons are explicitly resolved. This makes MD simulations one of the most used methods to measure thermal properties of materials, where heat is mainly transported by phonons. Unfortunately, the electronic contribution is neglected in MD, and thus, the study of materials where electronic heat transport is important cannot be performed with accuracy in MD. This render MD simulations well suited but also essentially limited to the simulation of low level of electronic excitation and ionization events, semiconductors and insulators. For example, phenomenon like swift heavy ion irradiation, short-pulse laser interaction, and metal–semiconductor joints where electronic energy loss/gain is significant cannot be accurately described using MD.

A preferred method to address this issue is the two-temperature molecular dynamics (2T-MD) model. In this approach, a Fourier law is used to describe the electronic energy transport and is combined with classical MD in a concurrent multiscale scheme. In this model, the temperature evolution in electronic subsystem is described by a heat diffusion equation \[ \frac{C_e}{\partial t} \frac{\partial T_e}{\partial t} = \nabla[K_e(T_e)\nabla T_e] - G(T_e - T_i), \] where \( C_e, K_e, T_e, \) and \( T_i \) are electronic heat capacity, thermal conductivity, local electronic and ionic temperature, respectively. \( G \) is a electron–phonon coupling constant between electron and phonons.

One appealing aspect of the 2T-MD model is that it can concurrently simulate energy exchange between electrons and phonons during a simulation. The implementation of equation (1) in MD codes has been achieved by a number of means, including finite differences (FDs) [5–8] and the finite elements method (FEM) [9]. In implementations using FD, the atomic system is divided into small cells (voxels) that generate a mesh and the FD method is used to evaluate the Laplacian of the electronic temperature and solve equation (1) for each voxel. Similarly, in implementations using FEM, the MD system is embedded into a FEM mesh, where some of the atoms generate the nodes of this mesh. Thus, the coupling is done by passing the MD simulation data into the FEM mesh, which solves equation (1). Other methodologies have coupled both phonons and electrons using a heat conduction equation as equation (1) while completely removing the lattice dynamics, leading to free-energy type methods to describe thermo-mechanical response of materials [10–14]. The 2T-MD approach has been successfully applied to multiple problems of technological interest such as strong electron–phonon non-equilibrium problems [15], laser ablation [16–18], shock induced melting [19], metals and semi-metals interfaces [20], energy transport across semiconductor–metal interfaces [21], and to irradiation damage of materials [22–27], to mention but a few. The reader is referred to the recent review by Darkins and Duffy for a perspective view of the model [28].

Regardless the choice of the method to evaluate the Fourier law for the electronic temperature, previous implementations have been using finite size sub-divisions of the system and linked the behavior of a cluster of atoms into the FD grid or FEM nodes. However, in many situations of interest, large temperature gradients appear in short length and time scales, and very fine spatial discretization of the electronic mesh is required to properly describe the temperature variation. This indicates that heavily excited atoms and electrons can quickly exchange energy in local regions of the system and thus, small resolution is required to resolve this issue. Hence, recent studies have been indicated the need for local 2T-MD methods that can accurately account for this [22, 23]. Additionally, in systems where liquid/solid interfaces appear, the amorphous nature of the atoms make it difficult to be described with accuracy using a voxel description or a FEM mesh.
In this work, we develop a new approach of the 2T-MD method by replacing the classical Fourier law by a Fokker–Planck equation to simulate the exchange of energy between electrons. The Fokker–Planck equation, used in the form of a master equation, computes the probability that two adjacent electronic sites exchange energy through electronic heat flow. This eschews the need of using an auxiliary mesh in order to evaluate the Laplace operator and retains, at the same time, the smallest resolution that one can achieve in MD systems, e.g. the atomic resolution. This is important as our approach can reproduce complex geometries in comparison with FD or FEM meshes. Another remarkable aspect of this approach is that by virtue of the master equation, the electrons exchange energy in a local fashion, which allows the application of our method to situations where the system is far from the thermodynamic equilibrium, e.g. large temperature gradients in small regions. Additionally, since the method does not need an auxiliary mesh, it can be seamlessly coupled to MD codes, and the electronic temperature can be easily initialized by assigning properties to the atoms, which reduces the effort of the users to define the coupled electrons-phonons system. Hence, we implemented the new method into the LAMMPS code \cite{29} and refer to it as \ell\textsuperscript{2T}-MD, and make it available through its online site \cite{30}.

The manuscript is organized as follows. First, we start by introducing the formulation and performing the energy balance to determine the coupling between electrons and phonons. Next, we demonstrate the methodology by using a simple one-dimensional (1D) example to simulate the electronic and phonon heat conduction using the traditional 2T model, and the master equation approach. Next, a one and two-dimensional (2D) models are used to study the coupling between electrons and phonons in MD system using the new implementation. We investigate the conservation of the energy in the system and the energy exchange between electrons and phonons. The parallel performance of the method is also studied. Finally, we study two problems of technological interest, an irradiation damage problem in Ni using a 50 KeV cascade simulations; and a laser spallation simulation in Ni. We conclude the manuscript with the main outcomes of this work.

2. Methodology

We now describe the \ell\textsuperscript{2T}-MD method. Let us now consider a system of \(N\) particles at finite temperature. This temperature is the contribution of two players, e.g. phonons and electrons. MD simulations explicitly model the phonons as a result of atomic interactions accounted for by the interatomic potential. Unfortunately, the electronic contribution to the temperature is neglected and difficult to model. The two-temperature model assumes that the temperature field can be split into two interacting subsystems, e.g. phonons and electrons. Thus, one has an electronic temperature, \(T_e\), and a lattice temperature given by the classical definition, i.e. \(T^{\text{lat}} = \frac{K}{2k_B N}\), where \(K = \sum_{i=1}^{N} \frac{1}{2} m_i v_i \cdot v_i\) is the total kinetic energy of the atoms, \(m_i\) and \(v_i\) are the mass and the thermal velocity of the \(i\)th-atom\(^1\), respectively, and \(k_B\) denotes the Boltzmann constant. We assume that associated with each atom, there is a local electronic temperature, i.e. \(T_e^{\text{local}}\) that can fluctuate from atom to atom. Noteworthy, this local electronic temperature field is clustering the contribution of many electrons surrounding the atoms. Let us now define the maximum \(T_e^{\text{max}}\) and minimum \(T_e^{\text{min}}\) allowed electronic temperatures in the system. Practically, \(T_e^{\text{min}} = 0\) K while \(T_e^{\text{max}}\) is selected sufficiently large such that the electronic temperature in the system does not exceeds this value. These values are kept constant

\(^1\) We define the thermal velocity as the instantaneous velocity minus the velocity of the center of mass, i.e. \(v_i = v_i^{\text{inst}} - v_{\text{com}}\), where \(v_{\text{com}} = \frac{1}{M} \sum_{i=1}^{N} m_i v_i^{\text{inst}}\), where \(M\) is the total mass of the system.
during a simulation. Introduce the normalized temperature field \( \theta_i^e = \frac{T_i^e - T_{\text{min}}^e}{T_{\text{max}}^e - T_{\text{min}}^e} \), which renders all normalized temperatures to the interval \( \theta_i^e \in [0, 1] \) \( \forall i = 1, 2, \ldots, N \).

Now, we are interested in simulating heat transport in MD simulations and include the effect of both phonons and electrons. In order to simulate heat conduction of the electronic temperature, we follow the approach proposed by Ponga and Sun [31] and modify it to consider coupling between electrons and phonons. Thus, we use the following modified master equation

\[
\frac{\partial T_i^e}{\partial t} = T_{\text{max}}^e \sum_{j=1}^{N_i} K_{ij}(\theta_j^e(1 - \theta_i^e) \exp[\Delta e_{ij}] - \theta_i^e(1 - \theta_j^e) \exp[\Delta e_{ij}]) - \frac{G}{C_e}(T_i^e - T_i^{l\text{th}}),
\]

where \( K_{ij} \) is a pair-wise exchange rate thermal coefficient for the electronic temperature \( [K_{ij} = \text{time}^{-1}] \), and \( \Delta e_{ij} = -\theta_j^e - \theta_i^e \) is the normalized difference in the electronic temperature between the \( i \)th and \( j \)th atoms, and \( C_e \) is the electronic heat capacity \( [C_e = \text{energy} \cdot \text{temperature}^{-1} \cdot \text{length}^{-3}] \). In our implementation, we use values of \( K_{ij} \) and \( C_e \) that are function of the temperature of the system. Temperature dependence of \( C_e \) and \( K_{ij} \) are calculated using simple linear relation of \( C_e = \lambda T_e \) and \( K_{ij} = \frac{\kappa_{ij} d}{T_e^2} \) where \( \kappa_{ij} \) is thermal conductivity at 273 K [32]. At each time step \( C_e \) and \( K_{ij} \) are calculated using the mean electronic and lattice temperature of the system. Linear dependencies of \( C_e \) has also been used before in other implementations of the 2T-MD model [5, 6, 33]. However, we notice that the linear dependence of the \( C_e \) and \( K_{ij} \) is an oversimplification, and more complex dependence can be implemented (see for instance [34–36]). We have implemented this temperature dependence using fifth degree polynomial interpolation to model the thermal dependence of \( C_e \) and power laws for \( G \). While some of the fine details change in the examples, the main mechanisms remain unchanged. Similarly, it is possible to define a local \( C_e \) and \( K_{ij} \) using the local electronic temperature in the model. These dependencies can be easily implemented in our code and some will be implemented in future versions of the code.

Let us now analyze the terms in equation (2) and their relation to heat conduction in the electrons. The first term on the right-hand side of equation (2) measures the rate of electronic energy exchanged between two adjacent particles and it is arbitrarily chosen to be around the nearest neighbors of the \( i \)th particle, which makes the model fully local. Practically, the user can specify a cutoff for this sum in the command, which should be slightly above the burgers vector in crystalline materials. However, it should be noted that extra neighbors can be selected and thus, rendering the model to a semi-local description. According to Ponga and Sun [31], the pair-wise exchange rate thermal coefficient can be computed from an asymptotic expansion of the master equation into the continuum limit leading to a relation with the (macroscopic) electronic thermal conductivity \( \kappa_{e} \) as

\[
K_{ij} = \frac{2\kappa_e d}{C_e Z b^2},
\]

where \( d \) is the dimension of the system, \( Z \) is the coordination number, \( b \) is the Burgers vector of the material.

The second term on the right-hand side of equation (2) is a linear coupling term between the electrons and phonons. \( G \) is a constant that defines the strength of the coupling between the atoms and the electrons and has units of \( [G = \text{energy} \cdot \text{length}^{-3} \cdot \text{temperature}^{-1} \cdot \text{time}^{-1}] \), and \( (T_i^e - T_i^{l\text{th}}) \) is the temperature difference between the electronic and lattice temperature of the \( i \)th particle. \( T_i^{l\text{th}} \) denotes the lattice temperature of the \( i \)th atom defined as
where \( v_j \) denotes the thermal velocity of the \( j \)th-atom. The \( j \)th-atoms are selected to be between a cut-off radius, i.e. \( j \in x_j - x_i \leq r_c \). In our work, the cut-off radius \( r_c \) is automatically selected to be the cut-off of the interatomic potential. The total number of particles in this cut-off radius is denoted by \( N_j \). It is worth mention that all MD codes already have a neighbor list generated in order to compute the atomic interactions. Taking advantage of this fact, we used the neighbor list of the atoms, that is efficiently generated by LAMMPS. As usual, the user is able to determine when to reconstruct this neighbor list.

After modeling heat conduction in the electronic system, we notice that the last term on the right-hand side of equation (2) is the amount of energy exchanged between electrons and phonons. This amount of energy needs to be introduced (removed) into (from) the lattice, and several alternatives exist to do this. There are several implementations of this term in the literature including the works of Duffy and Rutherford [6], Caro and Victoria [2], Finnis et al [3], Häkkinen and Landman [4], where the energy was inserted/removed by computing the amount of work that a random force will do in order to simulate a thermostat. An alternative approach is by modifying the equation of motion to include a damping force, i.e. Ivanov and Zhigilei [5]. For simplicity, our implementation followed the later approach. The amount of energy exchanged per unit of time and volume at the \( i \)th particle between the electrons and the lattice is \( G(T_e^i - T_{\text{lat}}^i) \). This flux of energy needs to be introduced (removed) in the lattice by modifying its kinetic energy. In order to do so, we introduce this energy flux by modifying the dynamics of the lattice, i.e.

\[
m_i \ddot{v}_i = F_i + F_{\text{damping}}^i = F_i + \xi_i m_i v_i,
\]

where \( \ddot{v}_i \) is acceleration of the \( i \)th-atom, \( F_i \) is the force acting on the \( i \)th-atom due to the interatomic interactions, and \( \xi_i m_i v_i \) is the damping force that appears due to the lattice heating (cooling) coming from the electronic temperature. \( \xi_i \) is a coupling coefficient of the \( i \)th-atom whose strength has to be computed at each time step. Let us now analyze the amount of energy exchange by the electronic temperature per unit of time. Letting \( V_{\text{atom}} = \frac{1}{N} \) be the atomic volume, the energy exchange between the lattice and the \( i \)th-atom is

\[
\frac{dE_{e-lat}^i}{dt} = GV_{\text{atom}}(T_e^i - T_{\text{lat}}^i).
\]

The rate of work (power) done by the damping force is

\[
W = v_i \cdot F_{\text{damping}}^i = \xi_i m_i v_i \cdot v_i.
\]

It is easy to see that \( \xi_i \) has to be computed at each time step in order to conserve energy in the system due to the exchange of energy between the electrons and the phonons. The rate work done by the damping force has to be equal to the amount of energy exchange by the electrons in equation (6), leading to

\[
\xi_i = \frac{GV_{\text{atom}}(T_e^i - T_{\text{lat}}^i)}{2K_i},
\]

where \( K_i = \frac{1}{2} m_i v_i \cdot v_i \) is the local kinetic energy of \( i \)th-atom. We notice that the quantity \( K_i \) could be instantaneously zero at certain time steps. This would lead to instabilities in the simulation, as the coupling coefficient will tend to infinity. This is due to the fact that the work done by the damping force tends to zero, and thus, even if \( \xi_i \) is large, it cannot
accommodate situations which ultimately affect the stability of the system. In order to avoid these numerical instabilities, we opted for avoiding energy exchange between phonons and electrons when $K_i < \epsilon$ at the $i$th-atom, where $\epsilon$ is a tolerance of $10^{-5}$ eV. This simple solution works well and does not affect the thermal behavior of the system.

Before closing this section, we make some remarks. First, we notice that the formulation uses local electronic and lattice temperature, and therefore, the energy exchange happens locally in the atoms. The strength of the coupling between electrons and phonons, given by $\xi_i$, changes atom by atom and it is a function of the time. Hence, in the current form, the electronic temperature serves as a local thermostat that tends to equilibrate the electronic and lattice temperatures. We also would like to point out that while in the current model it is numerically possible to assign a high electronic temperature to one atom, and a low electronic temperature to its neighbors, it is not physically meaningful since the framework will rapidly distribute—in a few femtoseconds (fs)—this large difference amongst its neighbor atoms. In our model, however, we are not assuming such scenarios, rather after the initial assignment, the temperature will evolve gradually and have some distribution over a wide range of electrons as we will see in the validation examples in the next sections. In our understanding and from the available literature, it is quite possible to have high electronic temperature gradient when ion energy is in electronic stopping range. Generally speaking, large gradients can exist in narrow areas although it might be very challenging to measure these conditions experimentally. For example, in swift heavy ion irradiation the initial energy is deposited in the electrons along the ion path until the nuclear stopping becomes dominant at low energy \[24, 37\]. Our technique allows such scenarios—for instance the irradiation damage and laser ablation examples—and these large gradients vanish very quickly.

2.1. Implementation

We have implemented the proposed $\ell^2$T-MD model in the LAMMPS code. We have done so by including an electronic temperature variable per atom. Then, the master equation equation (2) was implemented using a fix operation, which is called every integration step to evaluate the electronic temperature. The electronic temperature for each atom is updated using a user specified cutoff radius to select the nearest neighbors and can be selected from the input script file. Once the electronic temperature is updated, the coupling strength between phonons and electrons (equation (8)) is computed. Then, the force acting on the atoms is modified through equation (5) to include the damping force at the $i$th-atom. The fix was implemented to work for parallel calculations using the message passing interface library. Since the electrons thermal diffusivity is very high, the time step for the integration of equation (2) has to be a fraction of the integration time step in MD simulations ($\sim 1$ fs). Thus, during a lattice integration step, we actually allow to perform multiple integration steps of the heat equation, and this can be selected by the user from the simulation script. However, one must be careful since the electronic temperature in the ghost atoms that are not owned by the local process has to be updated at every electronic heat conduction step. Additionally, in large energy cascade simulations (>10 KeV), the velocity of the ions could be extremely high, and thus sometimes it is desirable to have a variable integration time step for the lattice. Our implementation is capable of handling this if the user specifies it. Cascade simulations described in section 4 were carried out using a variable time step. The source is an add-on to the LAMMPS code and can be found in its online site [30].
3. Heat conduction in Ni

3.1. 1D bar

Our first test consists of a classical two-temperature approach, where lattice and electronic temperatures are modeled. Our goal is to show the ability of the master equation approach to solve diffusion equation in a system of particles, and to compare it with the classical Fourier law. In order to do so, we solve a heat conduction problem in a 1D bar. In the classical two-temperature approach, a Fourier law is used to model simultaneously electrons and phonons heat conduction, i.e.

\[
\begin{align*}
C_e \frac{\partial T^e}{\partial t} &= \kappa_e \frac{\partial^2 T^e}{\partial x^2} - G(T^e - T^{\text{lat}}), \\
\rho C_{\text{lat}} \frac{\partial T^{\text{lat}}}{\partial t} &= \kappa_{\text{lat}} \frac{\partial^2 T^{\text{lat}}}{\partial x^2} + G(T^e - T^{\text{lat}}).
\end{align*}
\] (9a)

Our test consists in replacing the Fourier law used to model electronic heat conduction by the master equation while keeping the Fourier law for the lattice heat conduction. Thus, equation (9) (a) was replaced by the master equation (equation (2)). The equations were solved using a custom code in MATLAB. The mesh points coincided with the atomic positions, which were separated a distance \( b = \sqrt{2} a_0 / 2 \), where \( a_0 \) is the lattice parameter. The evolution of the lattice temperature was carried out using the FD method. In order to evaluate the Laplace operator of the temperature, we used a three-point FD stencil, and the temperature was integrated using a Euler forward algorithm. Periodic boundary conditions were enforced along the x-axis for both electrons and phonons.

Both electronic and lattice subsystems were kept at 300 K at the beginning of the simulation. For simplicity, a hot zone was created by applying 6000 K to the electronic subsystem to a span of length \( 2a_0 \) at the center of the bar. However, as mentioned early on, a distribution of temperature would be a more realistic condition. Nevertheless, the intention of this example is to compare the evolution of the traditional 2T approach with the proposed master equation, and thus, the simplified initial conditions used in the example are relatively easy to reproduce. Thus, this justify the choice of an initial high temperature in a narrow area. The dimensions of the Ni-bar was \( l_x = 100 a_0 = 25 \text{ nm} \), where \( a_0 = 0.3562 \text{ nm} \) is the lattice constant of fcc Ni. In the FD model, electronic temperature dependence was not considered for heat capacity \( (C_e) \) and electronic thermal conductivity \( (\kappa_e) \). The material constants used for the description of the electronic subsystem were, electron–phonon coupling \( (G) = 3.6 \times 10^{17} \text{ J m}^{-3} \text{ K}^{-1} \text{ s}^{-1} \), electronic heat capacity \( (C_e) = 3.6886 \times 10^5 \text{ J m}^{-3} \text{ K}^{-1} \) and thermal conductivity \( (\kappa_e) = 91 \text{ J s}^{-1} \text{ m}^{-1} \text{ K}^{-1} \) [5, 32] while for the lattice we took a fraction of it, specifically \( \kappa_{\text{lat}} = 0.05 \kappa_e \) [38]. These parameters were used to simulate Ni. The pair-wise exchange rate thermal coefficient \( K_{ij} \) was calculated using equation (3) with \( d = 1 \) and \( Z = 2 \). The lattice heat capacity \( (C_l) = 400 \text{ J Kg}^{-1} \text{ K}^{-1} \) and density \( (\rho) = 8890 \text{ Kg m}^{-3} \) were used for the lattice heat diffusion. A constant time step of 0.1 fs was used for both simulations.

The temperature profiles of the classical approach and proposed master equation model are shown in figures 1(a) and (b), respectively. In the figure, we observe how the heat is being diffused following a Gaussian profile for the electrons, as predicted by the analytical solution. The large thermal diffusivity of the electrons spreads the high temperature very quickly, as

\[ \text{In metallic materials, electronic thermal conductivity is much larger than the lattice one, and thus the reason for this assumption.} \]
can be seen in the graphical representation. Since the lattice thermal diffusivity is much smaller than the electrons, the rise of the lattice temperature is less evident and concentrated near the hot spot. We also notice that after 3 ps, both electronic and lattice temperature were in equilibrium, and a very good agreement between the two models is seen with only small differences in the electronic temperature. These differences can be due to discrepancies of the thermal conductivity in the models, as the pair-wise exchange rate given in equation (3) was obtained using a long wave analysis, and some small differences can be seen in this case, where the heat is being dissipated very fast. Besides these differences, we see that the equilibrium temperature at the end of the simulation is the same, an indication that the energy is conserved in the system. Next, we proceed to introduce electronic heat transport in MD simulations in the next example.

3.2. MD simulations

In this section, we describe a simple $\ell^2T$-MD model which is analogous to the previous one. We took a Ni-bar of dimensions $l_x = 25 \text{ nm}$—same as model above—and $l_y = l_z = 2\tilde{a}_0 = 0.71 \text{ nm}$. The $C_e$ and $K_{ij}$ were function of electronic temperature ($T_e$) as described in section 2, equation (3), using $\lambda = 1065 \text{ J m}^{-3} \text{ K}^{-2}$, $\left(\tilde{\alpha}_0\right) = 91 \text{ J s}^{-1} \text{ m}^{-1} \text{ K}^{-1}$, $d = 3$ and $Z = 12$. The integration time step of MD was 0.5 fs while the electronic one was ten times less. Thus, for each MD time step, we performed ten electronic heat conduction steps. Notice that even though the heat is being dissipated in one direction, our example is fully three-dimensional and no simplifications were made for the electronic heat diffusion.

Figure 2 shows the time evolution of the electronic and lattice temperature in the MD sample. The lattice temperature was computed by dividing the computational cell in individual bins along the $x$-direction, and computing the temperature of the atoms in that bin ($N_b$) for 20 time steps using the classical expression $T_{\text{lat}} = \frac{2K_e}{3N_b\tilde{a}_0^3}$. A value of $T_{\text{max}} = 20000 \text{ K}$ was used, sufficiently large to ensure a mapping the normalized temperature field to the segment.

One could, in principle, input the value of $K_{ij}$ using $Z = 2$ and $d = 1$—as in the 1D case—to obtain the same equilibration time as in the previous example. We have done so and the lattice and electronic temperature reach equilibrium about 3.2 ps, in good agreement with the previous example.
Figures 2(a)–(d) show the time evolution of the electronic and lattice temperature for \( \Delta t = 1, 2, 10, \) and 99.5 ps, respectively. We see that the electronic temperature was quickly distributed across the sample, as depicted in figures 2(a) and (b). However, after \( \Delta t = 10 \) ps, there were small differences between them due to poor lattice conductivity in Ni, with a larger lattice temperature in the middle of the sample where the initial hot spot was placed. After \( \Delta t = 99.5 \) ps, we observed that both temperatures were in equilibrium. Remarkably, once the system was in equilibrium, both electronic and lattice temperatures reached the same value, with some statistical fluctuations in the lattice temperature. The final mean temperature of both electronic and lattice subsystems reached equilibrium at \( \sim 350 \) K.

Figure 3 shows the snapshots of electronic temperature distribution of \( \ell^2 \)-MD simulation at different time steps. We see the ability of the model to retain an atomic resolution for the electronic temperature.

The percentage of energy partition of the \( \ell^2 \)-MD model is shown in figure 4. The total energy (TE) is conserved in the simulation. Initially, the energy in the electronic subsystem was around 2.55% of the total amount available in the system, while the potential and kinetic energy were 96.6% and 0.85%, respectively. However, as time went by, the energy was gradually transferred to the atomic subsystem; increasing both kinetic and potential energies, as can be seen in figure 4. We see that around \( \sim 5 \) ps, the energy partition remains more or less
stable until the end of the simulation. At this point, the electronic subsystem retained around 0.23% of the TE, while the potential and kinetic energy retained 98.76% and 1.01%, respectively.

Figure 5 shows the performance of the implementation in the LAMMPS code for the uniaxial bar problem with a larger number of atoms, i.e. $N = 40\,000$. As we can see, the implementation has good scalability up to 32 processors (80% efficiency). However, after this point, the communication becomes the bottleneck and the efficiency gets reduced ($\sim60\%$ for 96 processors). This is due to two main reasons, the number of atoms per processor reduces to less than 1000 atoms/processors, and therefore, it is difficult to scale since the ratio between
computing over communication time is reduced significantly. Second, in order to the electronic heat diffusion, we need to communicate information to the ghost atoms in the simulation, which is an overhead with respect to MD. Thus, this reduces the performance. Reduction of communication can be achieved by using hybrid implementations with threads in OpenMP, as was done before in other codes [39]. This will be addressed in the future.

3.2.1. Heat conduction in a thin film. Next, we proceed to illustrate the behavior of the system when the bar was changed to a plate. In this case, we selected a length $l_x = l_y = 50a_0$ and $l_z = 4a_0$. Periodic boundary conditions were used in x-and y-directions and free surfaces were simulated in the z-direction. Initially, we ran a traditional MD simulation until the lattice temperatures was in equilibrium at $T = 300$ K using the Canonical ensemble (NVT). The electronic temperature was also initialized to same value for all atoms. Then, an initial large value of the electronic temperature $T_e = 10,000$ K was given to all atoms in the region $6a_0 \times 6a_0$ in the center of the simulation cell. The material parameters were kept the same than the previous example.

In order to monitor the lattice temperature, we divided the simulation cell into $20 \times 20$ bins of equal size, and computed the lattice temperature every 0.5 ps for 20 time steps. With these values of the lattice temperature at each bin, we then performed a 2D spline interpolation to produce a smooth surface for visualization purposes. Figure 6 shows the time evolution of the electronic and lattice temperature in the simulation cell. Figures 6(a)–(c) show the electronic temperature for the atoms in the sample at different times. Clearly, the elevated temperature given to the central atoms was quickly dissipated across the sample, until the temperature was approximately constant after 20 ps. On the other hand, the lattice temperature, shown in figures 6(d)–(f) with the surface plots, gets diffused much slower than the electronic one, as can be seen in figures 6(e), where the central atoms were at about 450 K, to finally equilibrate with the electronic temperature at 20 ps at around 358 K. Remarkably,
the fluctuations observed in the lattice temperature are characteristic of the statistic nature of the temperature.

4. Irradiation damage modeling

Now, we turn our attention to simulate far from equilibrium phenomenon such as ion irradiation, where electronic excitations and ionizations are significant. Irradiation in metallic systems has been studied in several works including only the effect of the phonons [40, 41]. Here, we include the effect of the electrons and phonons using the proposed approach. We performed 50 KeV Ni cascade simulations to model irradiation induced damage of elemental Ni using two different models (classical MD and $\ell^2T$-MD). The cascade simulations were done using the newly implemented $\ell^2T$-MD method in LAMMPS [29] code. We used the embedded atom method based potential of Bonny et al [42] to model elemental Ni, however, the $\ell^2T$-MD method works with all potentials available in LAMMPS. This potential was developed to study the production and evolution of radiation defects, particularly, point defects. The simulation cell size was $34 \times 34 \times 34$ nm$^3$ containing $\sim 3500 \, 000$ atoms. The lattice and electronic subsystems were initially at equilibrium having a temperature of 300 K. Periodic boundary conditions were applied to all directions to mimic an infinitely large bulk system. The phononic system was cooled down at the boundaries using Berendsen temperature control and a Dirichlet/fixed boundary condition was used for the electronic system to 300 K. The electronic stopping was modeled as a friction force for atoms with kinetic energies higher than 10 eV and calculated using the stopping and range of ions in matter code version 2013 [43, 44]. A fixed time step of 1 (fs) was used to relax the system and a variable time step was used having the maximum time step restricted to 0.01 fs for cascade simulations. At the beginning of the simulation, a recoil energy of 50 KeV was given to a central atom at a random direction. A total of seven such simulations were performed to collect damage statistics, and each simulation was run at 300 K for 16 ps. Since heavily excited ions can traveled very large distances in short periods of time, we needed to reconstruct the neighbor list every 20 time steps in order to have the proper neighborhood of the atoms.
neighbor list was generated by LAMMPS, and we only specified the number of time steps at which it was reconstructed. We notice that this neighbor list was used for both the interatomic interactions obtained with the interatomic potential, and the master equation equation (2) to compute the electronic heat conduction.

The maximum electronic temperature was the highest atomic value calculated at the corresponding time step, which is shown in figure 7(a) as a function of time. It shows highly excited electrons in small regions that can reach temperatures in excess of 8000 K. We see that the maximum electronic temperature decreases very quickly and it reaches an equilibrium point at around 0.1 ps after the event. Now, let us turn our attention to the time evolution of the maximum lattice kinetic energy, shown in figure 7(b) where we have made comparison for regular MD and the ℓ²T-MD model. Two main key aspects can be observed from the figure. First, the rate of change of the kinetic energy is much faster for the ℓ²T-MD model, since the effect of electrons are taking into account and they contribute to dissipation. As a result, the maximum kinetic energy in the sample for the regular MD model remained large (∼15 KeV) for approximately 0.5 ps, while in the ℓ²T-MD model, the maximum kinetic energy was reduced immediately. More specifically, the kinetic energy in the ℓ²T-MD model was reduced from ∼35 KeV to ∼1 eV in around 2 ps while in the regular MD model this takes 3 ps. This affects the generation of defects, as we will explain later on. Second, the plot shows that local atoms in the sample were heavily excited as indicated by their kinetic energy and thus, were far from equilibrium in both MD and the ℓ²T-MD models.

Figure 8, shows the electronic temperature distribution of the 50 KeV recoil event after 0.02 ps together with atoms showing exceeding amounts of kinetic energy. We see that only a small fraction of atoms have kinetic energy in excess of 0.4 eV. However, the electronic temperature can reach exceedingly large values as shown in the color map. The rainbow color map shows a radial distribution of the electronic temperature on the plane, characteristic of a Gaussian type distribution. To have a better understanding of the temperature distribution, figure 8(b) shows the temperature distribution along the narrow slit (brown lines) on the plane shown in figure 8(a). We observed a large temperature gradient (∼250 K nm⁻¹) from the central hot zone to the surrounding. This is a clear indication of a large temperature gradient happening in a very small length scale, denoting the local character of the energy exchange in
the system. Our analysis illustrates the need for models that are able to have a fine resolution in order to properly predict the electronic effects in these situations.

Next, we focus our attention to the evolution of the damage in the sample. The Voronoi cell method was used to identify the final damage production [45]. In this method, Voronoi polyhedra were centered on each atom position in the ideal fcc crystal and compared with atoms in the defective crystal. Polyhedra with no atoms were labeled as vacancies and polyhedra with two or more atoms were labeled as interstitials. The total number of Frenkel pairs (FPs) are 90 ± 10 and 120 ± 12 for $\ell^2T$-MD and classical MD cascade simulations, respectively. The number of FPs and the standard error of the mean was calculated from seven simulations for each model. We see that even though the time evolution of the kinetic energy in the $\ell^2T$-MD model had very small differences with regular MD, the inclusion of electronic effects reduces the generation of FPs by 25% with respect to MD indicating that electronic effects should be taken into account when studying irradiation damage. The low number of FPs in $\ell^2T$-MD simulation is expected due to energy transfer to the electronic subsystem as shown in the kinetic energy plot (figure 7(b)). Figure 9 shows the final point defects of a representative classical MD simulation and the $\ell^2T$-MD simulation having same recoil direction. The features of cascade damage are well captured in the simulation. It is visible from the snapshot that the interstitials are more aggregated due to high mobility and diffusivity compared to vacancies.

5. Laser ablation

Laser simulations were performed by giving a Neumann boundary condition to the simulation cell. This boundary condition specifies the rate of change of the electronic temperature by giving a heat flow that follows the following expression [5]
Here, $i_0 = i(1-r)$ is the maximum absorbed intensity [temperature-time$^{-1}$], $(1-r)$ reflects the amount of energy absorbed, and $r$ is the reflection parameter, $x_i$ and $x_0$ are the first components of the position vector of the $i$th-atom and the free-surface end, where the laser pulse is applied, respectively. $l_p$ is the penetration length, $t_0$ is the time at which the pulse is applied and $\sigma$ is the standard deviation of the Gaussian profile.

In our simulations, we selected $i_0 = 10^5$ Kps$^{-1}$ (which gives a laser fluency of $F \approx 1320$ J m$^{-2}$), the half-width duration and the duration of the pulse were $\sigma = 1$ ps, and $\tau = 10.0$ ps, respectively. The penetration length was selected to be $l_p = 2$ nm. We notice that these parameters are arbitrarily selected for purposes of the example, and they might not be the best parameters to describe a particular laser wavelength. The simulation cell was $150a_0 \times 40a_0 \times 40a_0$ containing ~960 000 atoms, and it was carried out with a constant time step of $\Delta t = 5 \times 10^{-4}$ ps while the electronic time step was ten times smaller. The material’s constants and potential were specified in section 4.

In order to analyze the spatial and temporal evolution of the electronic and lattice temperature, and the stress in the sample, we divided the simulation cell in 40 bins of equal size along the $x$-direction. In each bin, we computed the averaged lattice temperature and stress. This values were used to understand the effect of the laser pulse in the sample in the next section.

5.1. Results

We first describe the time evolution of the lattice and electronic temperature across the sample. Figure 10(a) shows the spatial evolution of the electronic and lattice temperature for three different times. As we can clearly observe, they are in equilibrium at $t = 0$ ps. Some fluctuations appear in the lattice temperature due to the statistical nature of it. However, as the
Laser pulse was applied to the sample, the electronic temperature increased very rapidly in comparison with the lattice temperature, generating a non-equilibrium thermodynamic state. This can be seen in figure 10(b) where the electronic temperature is much higher than the lattice temperature. However, at around $t = 40$ ps, the electronic and lattice temperatures were very close to each other, with fluctuations less than 100 K.

In order to better visualize this, we plotted the evolution of the lattice temperature and the first component of the virial stress tensor, e.g. $\sigma_{xx}$, as a function of space and time. Putting space in horizontal axis, and time in the vertical one—the common way of studying wave propagation in materials—we generated the plots shown in figure 11. Focusing our attention

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**Figure 10.** Time evolution of the electronic and lattice temperature in the sample as a function of the position during the laser ablation simulation.

**Figure 11.** Space–time plots for the laser simulation. (a) Temperature as a function of space–time, and (b) stress as a function of space–time. The two dashed lines denote the spatial-temporal evolution of the new surfaces, while the dashed–dotted line indicate the portion of the atoms that has been melted.
on the spatial temporal evolution of the temperature (figure 11(a)), we see that the laser had a clear effect on the lattice temperature of the atoms placed near the left side of the sample. Their lattice temperature quickly increased up to \( \sim 2500 \) K in about 10 ps. On the other hand, for the atoms at the right end of the simulation, their temperature remained much lower, and is not until about 8 ps where the temperature increased about \( \sim 1000 \) K. At \( t = 10 \) ps, we see that the temperature profile has a large gradient, and the atoms near the left start to melt due to this large temperature. The dashed–dotted line delimits the fraction of atoms that has been melted during the laser heating. We see that the large energy deposited in the sample has an important effect on the sample, melting more than half the atoms in the sample in about \( t = 20 \) ps.

Nanovoids started to nucleate in the sample due to the melting process, and the large hydrostatic pressure generated by the heat wave. The initial moment in space and time where the first nanovoid was generated is highlighted with the letter A in figures 11(a) and (b). Thereafter, the number of nanovoids increased very quickly; eventually they coalesced and generated two new surfaces splitting the sample in two parts. The spatial and temporal evolution of the new surfaces is indicated with the two dashed lines in figure 11. Then, the temperature of the melted atoms oscillates between 1800 and 2100 K. For the atoms at the right-hand side of the cell, the temperature is below the melting point and remain in solid phase. Similarly, their lattice temperature was around 1000–1200 K, as shown in the figure.

Let us now focus our attention on the pressure evolution as a function of the space and time, depicted in figure 11(b). An initial compression wave was observed, denoted by a range of blue colors in the contour map shown in figure 11(b). We observed that this initial compressive wave travels approximately at the speed of sound in the material, and reached the end of the simulation cell at around \( t \sim 8.5 \) ps. Since the simulation cell was traction free at the free-surfaces, the compression wave reflected back as a tensile wave and traveled back to the sample. This generated a large tensile wave pulse where the stress reached exceedingly large values, which nucleated nanovoids. The location of the nanovoids is highlighted with the letter A in figure 11, which is near the middle of the sample, where the maximum tensile stress was achieved. Afterwards, multiple reverberations of a standing waves in the left side of the sample can be seen in the figure 11(b), as indicated by the negative and positive values of the stress evolution. We noticed that these values tended to decrease with time, due to dissipation mechanisms in the material. On the other side of the sample, similar behavior was seen, with the caveat that the values of the pressure were smaller. These results are in qualitative agreement with previous laser ablation simulations of Ni specimens carried out with the 2T-MD model \( [5, 16, 36] \).

Figure 12 shows the configuration of the sample and the electronic temperature for three different times, i.e. \( t_1 = 0.1, 16, \) and 22 ps. As can be seen in the figure, the laser pulse...
generated a large electronic temperature with temperatures in excess of 6000 K. In figure 12(b), we observed the nucleation of nanovoids in the simulation cell after $t = 16$ ps since the laser pulse started. These nanovoids grew very quickly and coalesced (figure 12(c)), generating a new surface and splitting the sample in two parts. In order to better visualize these nanovoids, we provide in figure 13 a surface reconstruction of the simulation cell at $t = 22$ ps after the laser pulse has been applied. We clearly observed several nanovoids nucleated in the sample, which eventually coalesced and generated two new surfaces.

We now turn our attention to the evolution of the virial stress in the sample as a function of time, and in particular to the hydrostatic component of it given by $\sigma_H = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$. This is shown in figure 14 where the hydrostatic and normal components of the stress tensor are shown. Figure 14 indicates that, initially, the laser pulse generated an overall compressive stress in the sample. The compressive pulse has its peak of $-7$ GPa at $t \approx 5$ ps. However, shortly after the peak compressive stress was reached, the
stress reduced and changed its sign at around $t = 8.7$ ps. The maximum tensile value of 4.5 GPa was reached at around $t \approx 12.5$ ps. The nucleation of nanovoids started at around $t = 16$ ps, and the coalescence of them at $t = 22$ ps, as indicated in the plot. After this time, the stress fluctuated with values that were bounded by the maximum compressive and tensile values.

The evolution of the local structure of the atoms was also monitored using the common neighbor analysis algorithm [46]. At $t = 0$ ps, the sample contained mainly fcc atoms (99.9%) and few atoms in other types due to surface effects (0.1%). As the laser pulse injected energy to the sample, the fraction of atoms in amorphous phase increased almost linearly until $\approx 62\%$ of the atoms becomes amorphous at $t = 12.5$ ps, which coincided with the maximum peak stress. Thereafter, the portion of the atoms in amorphous phase remained the same, and mainly located in the left-hand side of the images shown in figure 12, where the laser pulse was applied.

We finally investigated the partition of the energy as a function of time during the laser simulation. The time evolution of the partition of the energy is shown in figure 15. Initially, at $t = 0$ ps, the potential energy had 99% of the energy in the sample, and the kinetic energy was around 0.9%. The electronic subsystem had 0.1% of the energy. Once the laser pulse was applied to the sample, the distribution of the energy changed drastically, as can be observed from the figure. The maximum share of electronic energy was achieved at $t = 1.75$ ps, where the electronic subsystem had 27.97% of the energy, while the potential and kinetic energy had 70.60% and 1.43%, respectively. Thereafter, the laser pulse decrease its intensity and a complex process of energy exchange initiated. As a result, the potential and kinetic energy increased rapidly, and around $t = 20$ ps the distribution was 90.23%, 4.66%, and 5.11% for the potential and kinetic energy, and the electronic subsystem, respectively. After this point, small fluctuations were observed, but the numbers remain in the same ballpark until the end of the simulation. The partition of the energy indicate that the laser-photons-interact in a very short time scale with electrons, and then electrons transmit part of the energy to the lattice,
generating structural changes, and multiple waves emission due to the non-equilibrium state generated by the laser pulse.

6. Conclusions

We have developed, implemented, and validated a new approach, called ($\ell^2$T-MD), of the two-temperature model coupled with MD simulations into the LAMMPS code. The methodology uses a master equation to compute effective rates of energy exchange in the electronic subsystem and it is coupled to the phonon vibrations of the atoms through classical MD. We have demonstrated the new methodology through multiple examples of technological relevance.

In the cascade simulations, we found that while the mean average electronic temperature remains relatively small, the maximum temperature in the system can reach exceedingly large values. For instance, in the 50 KeV simulation, the mean electronic temperature increased up to $\sim$450 K, while the maximum reached about $\sim$8000 K. We also showed that the temperature gradients can be very large, of the order of $\sim$250 K nm$^{-1}$, as demonstrated in the electronic temperature across a section of the simulation. Such a large gradients illustrates the ability of the master equation and the current approach to transport energy at the atomic scale including situations where the system is far from the thermodynamic equilibrium while retaining the smallest discretization possible in classical atomistic systems. Interestingly, the introduction of electrons in the irradiation damage simulations leads to a significant reduction of the numbers of FPs with respect to MD, illustrating the need for including electronic effects. We also illustrated a laser ablation simulation, where a large amount of energy was introduced in the sample, generating melting of the sample, nanovoid nucleation, growth and coalescence of voids, leading to separation of the material.

The current approach provides a mesh free alternative for coupling electrons with phonons in MD softwares. This is important because the implementation can be seamlessly implemented in multiple MD codes. We have done so using the LAMMPS code, providing capabilities for simulating atomic systems with massively parallel clusters. The implementation can be downloaded from its web site [30].

Before closing, we would like to mention that the classical 2T-MD does not take into account quantum mechanics effects, such as magnons temperature and complex interactions between electrons and phonons. Thus, in that sense, the proposed $\ell^2$T-MD model can be further improved to include more physics, such as the coupling of electrons and phonons with magnons to simulate ferroelectric materials, ballistic effects in electrons, and more complex coupling models between electrons and phonons, specially in the high temperature range, where the coupling strength can change in a nonlinear fashion [28, 38, 47]. We believe that these shortcomings can be addressed in the future by modifying the master equation to include magnons’ temperature, ballistic effects, and more complex coupling between electrons and phonons. In particular, the combination of non-equilibrium ab initio methods can be used in conjunction with the $\ell^2$T-MD model to describe complex phenomena that cannot otherwise be simulated with state of the art ab initio nor MD methods.

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