Modelling of dislocation generation and interaction during high-speed deformation of metals.*

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Abstract

Recent experiments by Kiritani \textit{et al.} \cite{Kiritani} have revealed a surprisingly high rate of vacancy production during high-speed deformation of thin foils of fcc metals. Virtually no dislocations are seen after the deformation. This is interpreted as evidence for a dislocation-free deformation mechanism at very high strain rates.

We have used molecular-dynamics simulations to investigate high-speed deformation of copper crystals. Even though no pre-existing dislocation sources are present in the initial system, dislocations are quickly nucleated and a very high dislocation density is reached during the deformation.

Due to the high density of dislocations, many inelastic interactions occur between dislocations, resulting in the generation of vacancies. After the deformation, a very high density of vacancies is observed, in agreement with the experimental observations. The processes responsible for the generation of vacancies are investigated. The main process is found to be incomplete annihilation of segments of edge dislocations on adjacent slip planes. The dislocations are also seen to be participating in complicated dislocation reactions, where sessile dislocation segments are constantly formed and destroyed.

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1 Introduction

In a recent paper, Kiritani et al. reported that a large number of vacancies were produced during high-speed heavy plastic deformation of thin foils of fcc metals [1]. They observed a large density of stacking-fault tetrahedra but very low dislocation densities in the foils after deformation. As a possible explanation, they propose a dislocation-free deformation mechanism.

In this paper we investigate the deformation processes in metals under very high strain rates. Our approach is that of Molecular Dynamics (MD), where Newton’s second law is solved numerically for all the atoms in the system under consideration. The main advantage of this method is that no a priori assumptions are made about the deformation mechanism. Structures such as dislocations appear automatically from the motion of the atoms. The simulation thus becomes “unbiased”, i.e. the result is independent of our prior assumptions about the active deformation mechanisms.

We have chosen to simulate the deformation processes in systems that are initially dislocation-free (i.e. without conventional dislocation sources such as Frank-Read sources). We start with single crystals in order to avoid dislocation emission from grain boundaries. Simulations of high-speed deformation of polycrystalline (nanocrystalline) material have been reported elsewhere [2, 3, 4]. Although many metals were studied experimentally by Kiritani et al. [1], we have chosen to focus our simulations on one metal: copper.

2 Simulation methods and setup

In order to get meaningful results from a molecular dynamics simulation, it is essential that the interatomic forces used in the simulation are a good approximation to the forces the atoms would experience in a real physical system with the same atomic configuration. We use the effective medium theory (EMT) [5, 6] to describe the interatomic interactions, as the EMT potential for copper has been well tested.

The simulated systems were single crystals. Two different system sizes were used, one with approximately 95,000 atoms and one with approximately 765,000 atoms. The linear dimensions of the two systems are approximately 10.5 nm and 21 nm. In both cases periodic boundary conditions were applied to the simulation, so the system effectively becomes an infinite crystal.

In the smaller system four vacancies were created in the initial configuration, by removing four random atoms. They were introduced in the unlikely case that vacancies were somehow actively participating in the deformation. The system is deformed along the [521] direction at a temperature of 450 K. We have chosen this temperature since we consider it likely that significant local
heating is occurring in the experiments due to the high strain rate.

As the preexisting vacancies in the smaller system did not participate in the deformation, no vacancies were introduced in the larger system. It was deformed along the [105] direction at the same temperature.

The systems were deformed at a constant strain rate, while keeping the stress in the transverse direction approximately constant. This procedure is further described in ref. [3]. In all cases a strain rate of $10^9 s^{-1}$ was used (compared to approximately $10^5 s^{-1}$ in the experiments). To keep the temperature of the system approximately constant during the simulation, Langevin dynamics [7] are used, i.e. a friction and a fluctuating force are added to the equations of motion of the atoms. We use a timestep of 5 fs, safely below the value where the dynamics becomes unstable.

During the simulations, configurations were rapidly quenched, and the local crystal structure was identified by common neighbor analysis [8, 9]. This was used to generate plots where all atoms except atoms at the dislocation cores were made invisible, allowing the visualization of the dislocation structures.

### 3 Results

Figure 1 shows the deformation of the smaller system. In figure 1(b) the first dislocation activity appears in the form of a few dislocation loops. The loops are nucleated homogeneously, i.e. without the presence of dislocation sources or crystal defects. The exact time and position of the nucleation event is determined by random thermal fluctuations. The loops are faulted loops consisting of a single partial dislocation with a stacking fault inside the loop. The loops expand rapidly. Due to the periodic boundary conditions the dislocations cannot disappear from the sample. They will continue to move causing significant plastic deformation. As the dislocations on different glide planes interact, dislocation reactions occur and a number of triple junctions appear. These typically consist of two Shockley partials that meet to form a stair-rod dislocation. Continuous formation and destruction of these sessile dislocations are seen in the simulations.

The dislocations observed in the simulations are mainly single Shockley partials. The homogeneous dislocation nucleation mechanism makes it very difficult to nucleate the second partial. Dislocations are only nucleated at extremely high stresses, but as soon as the first partial dislocation is created, it locally shields the stress field and prevents the second partial from nucleating. It probably also plays a role that the stacking fault energy is low. At high stresses the energy

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1Copper has a relatively low stacking fault energy, and furthermore the stacking fault energy in the simulation is approximately a factor of two below the experimental value (30 mJ/m² versus 52 mJ/m²).
Figure 1: System I. In this and the following figures only atoms near crystal defects are shown. Eight lighter gray atoms indicate the corners of the simulation cell. In part (a) the four initial vacancies are seen. The vacancies themselves are not shown, but the 12 atoms next to the vacancies are shown, as they are missing a nearest neighbor and therefore have the coordination number 11. In part (b) the first dislocation activity is seen. Part (c) shows the first generation of vacancies, and part (d) shows the final configuration, where a high density of vacancies is seen.
of the stacking faults become small compared to other energies in the system, such as the energy released by a moving dislocation.

After some dislocation activity has occurred we observe the first creation of vacancies in figure 1(c). A “sausage-like” string of vacancies has appeared in the middle of the system. Further dislocation activity breaks up the string of vacancies into smaller clusters.

To analyse the process by which such a cluster of vacancies is generated, we repeated the relevant part of the simulation, using a higher time resolution for the analysis of the process. This revealed the detailed process generating these vacancies. The mechanism is illustrated in figure 2. Dislocation interactions have created dislocations where segments are on different glide planes. This makes it possible for a segment of a dislocation to be annihilated. If two edge dislocations gliding on adjacent glide planes annihilate, a string of vacancies is formed. This appears to be the main source of vacancies in the simulations.

At the end of the simulation (figure 1(d)) a large number of vacancies have been formed, apparently by this mechanism.

The larger system behaves in a similar fashion. Figure 3 shows the larger

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If the dislocations had the opposite signs, a string of interstitials should be formed. This is not observed in the simulations, probably because the energy of such a string is too high, so the dislocations pass each other instead of annihilating.

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Figure 2: The vacancies are generated by the annihilation of two segments of edge dislocations. Left: The configuration just before the annihilation. A short segment of an edge dislocation is meeting an edge dislocation with the opposite Burgers vector. They are gliding on adjacent (111) planes. One of the dislocations is switching glide plane at two point along the dislocation line, as the dislocation is moving stair-rod dislocations are left behind. Right: The dislocations have collided and a small dislocation loop has been separated from the rest. The dislocation loop quickly collapses to a string of vacancies.
system after the deformation. As a large number of dislocations were present, it would have been very difficult to see anything in the figure if the entire system were plotted. For this reason only a slice through the system is shown. Again a large number of both dislocations and vacancies are seen.

### 4 Discussion

The simulations presented here indicate that the deformation of fcc metals at ultra-high strain rate occurs by mechanisms that are not very different from what is seen at more moderate strain rates. Even in a situation where there are no preexisting dislocations, and no dislocation sources, dislocations are nucleated and are the main carriers of the deformation. The main difference between the deformation mechanism in the simulations and in slowly deforming materials is how the dislocations are nucleated. This difference may not be present in a real physical sample under ultra-high-speed deformation, since dislocation sources
will be present, even though it is possible that other types of dislocation sources are activated under high strain rate conditions.

The high concentration of vacancies in the simulations is due to the very high dislocation density during the high-speed deformation. As the vacancies are generated when opposite-signed dislocations collide, it must be expected that the generation rate depends on the dislocation densities obtained and not just on the total deformation. It is therefore expected that much higher vacancy densities should be observed experimentally after ultra-rapid deformation than after deformation with moderate strain rate.

In the simulations presented here there are no free surfaces, and no efficient way of removing dislocations except by annihilation. We therefore expect a higher dislocation density and a higher vacancy production rate than those which would be observed with a more realistic geometry.

To test the effect of free surfaces, we have made a similar simulation with four free surfaces (i.e. the system has the form of a rod being pulled). In this case dislocations were nucleated at the corners, passed through the system and disappeared at the free surfaces on the other side of the sample. Only a few dislocations were moving through the system at the same time. No vacancies were generated, as the dislocations never collided. Preliminary simulations with two free surfaces (i.e. foil geometry) indicate that this geometry behaves much like the bulk simulations, as dislocations perpendicular to the surfaces cannot move to the surface and disappear. A large dislocation density builds up, and vacancies are generated.

5 Conclusions

Atomic-scale computer simulations using molecular dynamics indicate that ultra-high-speed deformation of fcc copper occurs by the nucleation and motion of dislocations. Even in the absence of dislocation sources, dislocations will be nucleated at sufficiently high stresses.

During the deformation, a large number of vacancies are formed, in agreement with experimental investigations of ultra-high strain rate deformation of thin foils of fcc metals [1]. The vacancies are produced when segments of edge dislocations moving on adjacent slip planes annihilate. This generates “strings” of dislocations. Further dislocation activity tends to break these strings into smaller clusters. Finally, over time spans much longer than those which we can simulate using molecular dynamics, the vacancies will diffuse and will eventually cluster, forming stacking fault tetrahedra.
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