Molecular Dynamics Modeling of Crack Propagation

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Abstract. The study is focused on the application of different approaches for initial crack propagation angle determination. Copper plate with the central crack under complex mechanical stresses (Mode I and Mode II loading) is studied by extensive molecular dynamics simulations using EAM potential. In addition, the complete Williams expansion for the crack tip fields containing higher-order terms is used. Crack propagation angle is obtained by 1) multi-parameter fracture mechanics approach based on three fracture mechanics criteria, MTS, maximum tangential strain and SED; 2) atomistic modeling for mixed-mode loading of plane medium with the central crack. From our simulations we can derive crack propagation directions and crack angles. MD calculations were run for three different values of the mixity parameter: 0.4, 0.5 and 0.6. Calculated values of crack angles were -51.5°, -46.6° and -42.2° accordingly. All the fracture criteria tested give similar values of crack growth angle for different values of the mixity parameter. It is shown that initial crack propagation angles given by both approaches are very close, especially when higher order terms of Williams series expansion for stress/displacement field description are taken into account. Thus, one can conclude that the criteria of classical continuum mechanics MTS and SED can give satisfactory predictions for crack initiation direction. Crack propagation direction angles given by conventional fracture mechanics reasonably agree with the angles obtained from molecular dynamics simulations.

1. Introduction

Thorough study of nonlinear deformation and fracture processes and nonlinear mathematical models describing these processes is done, as a rule, with the help of numerical computational experiment [1]-[9]. Among the approaches for crack propagation modeling, molecular dynamics method (MD) gives significant advantages in plastic deformation modeling [8]-[9]. While other computational methods describe subject matter using continuous equations, MD allows one to model selected set of atoms individually. This approach can predict and describe occurrence of particular plastic defects, vacancies and deformations. Thermodynamic and mechanical properties of specimen can be obtained via additional computations and analysis. The purpose of this research is central crack propagation modeling in monocrystalline copper in full range of mixed mode loading, from pure mode I to pure mode II loadings. Calculations were made using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[10] at wide range of starting temperatures, from 0.1K to 150°C. Whole process of crack development is observed and analyzed with the help of visualization tools and additional Python code. Trajectories and crack propagation angles are obtained for different mixed-mode loadings.

2. Mechanical properties

Internal structure of crystals plays significant role in mechanical behavior of metal. There are several crystal structures of monocrystalline copper with different lattices, lattice parameters and symmetry groups [11].
Table 1. Crystal structures of copper.

| Formula | Spacegroup | Formation Energy (eV) | Volume | Density | Crystal system |
|---------|------------|-----------------------|--------|---------|----------------|
| Cu      | Fm\(\overline{3}m\) | 0                     | 11.872 | 8.888  | cubic          |
| Cu      | P6\(_3/mmc\) | 0.004                 | 47.264 | 8.93   | hexagonal      |
| Cu      | P6\(_3/mmc\) | 0.006                 | 23.617 | 8.936  | hexagonal      |
| Cu      | Im\(\overline{3}m\) | 0.035                 | 11.853 | 8.903  | cubic          |
| Cu      | I4/mmm     | 0.035                 | 11.875 | 8.886  | tetragonal     |
| Cu      | Cmcm       | 0.15                  | 24.777 | 8.518  | orthorombic    |
| Cu      | P\(\overline{3}m1\) | 0.158                 | 138.316 | 4.577 | trigonal       |
| Cu      | P2\(/m\)   | 1.942                 | 603.475 | 0.175 | monoclinic     |

As it is shown in Table 1, there are two dominant systems of copper crystals with lowest possible energy: cubic (FCC) and hexagonal (HCP). Other crystal systems require very high energy per atom to occur in chosen set of temperatures and pressures. We calculated mechanical properties of these two systems in LAMMPS. Let’s denote position of a given atom in a cell as \(r\). In relative coordinates:

\[
L_p = \begin{pmatrix} l_1 \\ l_2 \\ l_3 \end{pmatrix} = \begin{pmatrix} l_{1x} & l_{1y} & l_{1z} \\ l_{2x} & l_{2y} & l_{2z} \\ l_{3x} & l_{3y} & l_{3z} \end{pmatrix},
\]

\[V = \text{det}(L_p)\].

Here \(l_1, l_2, l_3\) are fundamental vectors of a primitive cell, \(h\) is a vector in relative coordinates, \(V\) is a volume of a cell. During elastic deformations new coordinates are obtained:

\[
r' = hL_p^\prime \rho,
\]

\[V = \text{det}(L_p^\prime)\].

Potential energy of a cell can be expanded in a Taylor series:

\[E(\epsilon) = E(0) + \sum_{i}^{6} \frac{\partial E}{\partial \epsilon_i} \epsilon_i + \frac{1}{2} \sum_{i,j}^{6} \frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j} \epsilon_i \epsilon_j.\]

Here we use Voight notations, and \(E(0)\) is the energy of orginal cell equilibrium state and \(\epsilon\) is a deformation. Knowing, that \(C_{ij}\) can be calculated as

\[C_{ij} = \frac{1}{V} \frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j},\]

we can obtain stiffness tensor using different combinations of deformations, minimizing energy of a deformed cell using conjugated gradiend method. Minimal energy state is required to eliminate the second term in Taylor series.

Once stiffness tensor is obtained, one can calculate distribution of Young’s modulus at different angles.

\[E = (a_ia_ja_ka_lS_{ijkl})^{-1}, \quad a = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix},\]

Here \(S_{ijkl}\) is a compliance tensor, \(S_{ijkl} = C_{ijkl}^{-1}\).
2.1. FCC copper

FCC (face-centered cubic) crystal structure of copper is considered default for molecular dynamic calculations.[14] Most of many-body potentials (EAM or mEAM, for example) will work only with this crystal structure [15]. We calculated stiffness tensor $C_{ij}$ for this crystal and extracted elastic parameters. We compared our results with material properties from [11], [12]

\[
\begin{pmatrix}
185 & 123 & 123 & 0 & 0 & 0 \\
123 & 185 & 123 & 0 & 0 & 0 \\
123 & 123 & 185 & 0 & 0 & 0 \\
0 & 0 & 0 & 80 & 0 & 0 \\
0 & 0 & 0 & 0 & 80 & 0 \\
0 & 0 & 0 & 0 & 0 & 80 \\
\end{pmatrix}
\]

|                | Average values          |
|----------------|-------------------------|
|                | Bulk Modulus            | 145 GPa |
|                | Young’s Modulus         | 136 GPa |
|                | Shear Modulus           | 51 GPa  |
|                | Poisson’s ratio         | 0.34    |
|                | Elastic Anisotropy      | 1.51    |

**Figure 1.** Young’s modulus of FCC Cu.  
**Figure 2.** Shear modulus of FCC Cu.

Figures 1 and 2 show distribution of Young’s modulus and shear modulus at different directions, respectively. FCC structure gives surprising amount of anisotropy. As one can see from Figure 2, FCC copper has preferred directions of shift at around 45° in XY-plane. That can explain predominance of this direction in our previous calculations [7] of crack propagation direction angles. But crack tip quickly accumulates enough energy per atom for structural transition from FCC to HCP crystal structure with different Young’s modulus and shear modulus distributions.

2.2. HCP copper

HCP (hexagonal closed packing) crystal structure of copper is described only by selected set of atomistic potentials, mostly developed from modifying EAM files for FCC copper [16]. Once again, stiffness tensor $C_{ij}$ was computed for given crystal structure, yielding different distribution of elastic properties.
Stiffness Tensor of HCP Cu

\[
\begin{bmatrix}
211 & 119 & 101 & 0 & 0 & 0 \\
119 & 211 & 101 & 0 & 0 & 0 \\
101 & 101 & 263 & 0 & 0 & 0 \\
0 & 0 & 0 & 41 & 0 & 0 \\
0 & 0 & 0 & 0 & 41 & 0 \\
0 & 0 & 0 & 0 & 0 & 50 \\
\end{bmatrix}
\]

Average values

- Bulk Modulus: 142 GPa
- Young’s Modulus: 130 GPa
- Shear Modulus: 48 GPa
- Poisson’s ratio: 0.35
- Elastic Anisotropy: 0.35

Figure 3. Young modulus of HCP Cu.

Figure 4. Shear modulus of HCP Cu.

Figure 4 shows less anisotropy of elastic properties and can give wider range of crack propagation direction angles. At lower mixities, closer to mode II ($M^e = 0$), we observe more frequent structural transitions and thus angles, different from 45°, as it is predicted by Williams expansion.

3. Computational details

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[10] was used for molecular dynamics calculations. Computational cell contained from 30 thousand to 15 million atoms. Small scale models were used in calculations of elastic properties. All specimens were preserved in Nose-Hoover thermostate using grand canonical (NVT) ensemble. At every step pressure and temperature of the system and every atom are calculated [13]. Embedded Atom method is used to calculate energies of atomic interactions. Positions and velocities are updated using Newtonian equations of motion.

Temperature of the cell can be computed from:

\[
T = \frac{2}{3Nk_b} \sum_{i=1}^{3N} \frac{p_{i\alpha}^2}{2m} = \frac{2}{3Nk_B} \sum_{i=1}^{3N} \frac{m r_{i\alpha}^2}{2}.
\]

Pressure and stress are obtained from next equations:

\[
P = \frac{NkT}{V} - \frac{1}{3V} \left( \sum_{i=1}^{N} \sum_{j<i} \frac{\partial V_i(r_{ij})}{\partial r_{ij}} \cdot r_{ij} \right),
\]
\[ (\sigma)_{\alpha\beta} = -\frac{1}{V} \left( \sum_{i \in V} m_i v'_{i\alpha} v'_{i\beta} + \frac{1}{2} \sum_{i \in V} \sum_{j \neq i} f_{ij}^{\alpha} x_{ij}^\beta \right). \]

4. Results

Results show crack growth along XY plane at different timesteps. OVITO visualization tool was used to show stress accumulation at crack tips. Brighter colors represent higher amounts of stress.

**Figure 5.** fcc-Cu, initial configuration.

**Figure 6.** fcc-Cu, 23 ps.

**Figure 7.** fcc-Cu, 36 ps.

**Figure 8.** fcc-Cu, 45 ps.

Figures 5-8 show forces per atom, while figures 9-12, and 13-16 show $\sigma_{xx}$ and $\sigma_{yy}$ respectively.

**Figure 9.** hcp-Cu, initial step.

**Figure 10.** hcp-Cu, 4 ps.

**Figure 11.** hcp-Cu, 12 ps.

**Figure 12.** hcp-Cu, 16 ps.
Temperature distribution is shown in figures 17-20.

Figure 13. hcp-Cu, initial step.

Figure 14. hcp-Cu, 4 ps.

Figure 15. hcp-Cu, 12 ps.

Figure 16. hcp-Cu, 16 ps.

Figure 17. hcp-Cu, initial step.

Figure 18. hcp-Cu, temperature at 12 ps.

Figure 19. hcp-Cu, temperature at 14 ps.

Figure 20. hcp-Cu, temperature at 16 ps.

Average temperature of the specimen is shown on 21 and 22. $\sigma - \epsilon$ dependance is given in figures 23, 24.
5. Conclusions
Molecular dynamics calculation of crack a plane with central crack is performed. Mechanical properties of crystalline HCP and FCC copper show good correspondence with other experimental and theoretical results [14]-[16]. Elastic anisotropy is analyzed. Temperature impact is factored in atomistic model and heat distribution is obtained. Crack direction angles are computed. These angles are close to angles obtained from finite element method calculation and Williams series expansion.

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