Excitation of characteristic modes of a crystal during solid fracture at high tensile pressure

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Abstract. We have performed uniform triaxial deformation of single crystal copper at high strain rate using molecular dynamics code LAMMPS. The best-fit void nucleation and growth parameters are obtained using a macroscopic nucleation and growth (NAG) model. The detailed analysis of the data shows that voids nucleate at specific locations in the domain, and subsequently grow and coalesce. We explain the spatial location of first void nucleation in terms of the excitation and interaction of characteristic modes in the crystal domain using singular value decomposition analysis.

1. Introduction

High-velocity impact involving metals produces high tensile pressures in a small region. The resulting nucleation, growth and coalescence of voids lead to spall. Existing fracture models at high strain-rates, such as the Nucleation and Growth (NAG) model [1], involve several parameters, best-fit values of which are required for different materials. These best-fit parameters are available in the literature only for a few materials. If some of these parameters can be obtained from atomistic simulations, others can be determined by comparison with the experiment, e.g. spall produced by plate impact. In our earlier work [2], we have performed uniform triaxial deformation of crystal copper at $5 \times 10^9$/s strain rate and best-fit void nucleation and growth parameters are obtained for NAG model.

In the present work, we perform singular value decomposition analysis to determine the characteristic modes excited in the system, including their frequencies and associated distortions and attempt to explain the locations where nucleation first takes place.

2. Computational Method

Uniform triaxial deformation of single crystal copper has been performed at $5 \times 10^9$/s strain-rate using molecular dynamics (MD) code LAMMPS [3]. We have used embedded-atom method potential parameters generated by Foiles et al [4] for this study. Periodic boundary conditions are applied along all three directions. Simulation domain contains 360 atoms corresponding to $10 \times 3 \times 3$ unit cells. The system is first relaxed to 300 K and 1 bar pressure using an NPT simulation. The equations of motion are integrated with a time step of 1 femto-second using the velocity-Verlet algorithm.
3. Singular Value Decomposition (SVD) Analysis

3.1. Introduction

Details of the singular value decomposition analysis are described in [5]. A brief description of the method is presented here. In this technique, a matrix $A_{m \times n}$ is decomposed into three new matrices:

$$A_{m \times n} = U_{m \times m} S_{m \times n} V^T_{n \times n}$$  \hspace{1cm} (1)

where $UU^T = I$, $VV^T = I$ (i.e., $U$ and $V$ are orthogonal matrices); the columns of $U$ are the orthogonal eigen vectors of $AA^T$, the columns of $V$ are the orthogonal eigen vectors of $A^T A$ and $S$ is a diagonal matrix containing the square roots of eigen values from $U$ or $V$ in descending order.

3.2. Application to MD output

Matrix $A_{M \times N}$ generated from MD output is given as follows:

$$A_{MN} = \begin{bmatrix}
A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\
A_{21} & A_{22} & A_{23} & \cdots & A_{2N} \\
A_{31} & A_{32} & A_{33} & \cdots & A_{3N} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
A_{M1} & A_{M2} & A_{M3} & \cdots & A_{MN}
\end{bmatrix}$$  \hspace{1cm} (2)

where $M$ is the number of time steps for which atomic positions are output and $N = d N_{atoms}$, where $N_{atoms}$ is the number of atoms used in the MD simulation and $d$ is the dimension of the system. Therefore, we can write

$$A_{11} = x_{11}, A_{12} = y_{11}, A_{13} = z_{11}; A_{14} = x_{12}, A_{15} = y_{12}, A_{16} = z_{12}, \ldots$$

Rewriting the above matrix (Eq. 2) as follows:

$$A_{MN} = \begin{bmatrix}
x_{11} & y_{11} & z_{11} & \cdots & x_{1N} & y_{1N} & z_{1N} \\
x_{21} & y_{21} & z_{21} & \cdots & x_{2N} & y_{2N} & z_{2N} \\
x_{31} & y_{31} & z_{31} & \cdots & x_{3N} & y_{3N} & z_{3N} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
x_{M1} & y_{M1} & z_{M1} & \cdots & x_{MN} & y_{MN} & z_{MN}
\end{bmatrix}$$  \hspace{1cm} (3)

here $x$, $y$ and $z$ are the atomic positions. Decomposition of this matrix using SVD gives information on temporal variations of atoms ($U$), information on spatial correlations amongst the atoms ($V$) and the amplitude ($S$) of the modes excited in the system. As discussed above, the singular values ($S$ values) which are the representative of the amplitude of modes are arranged in descending order which means that even fairly weak modes excited in the system can also be identified.

4. Results and Discussion

Using the atomic coordinates output every 5 femto-seconds, we have performed the SVD analysis [6] to determine the characteristic modes excited in the system during deformation.
4.1. Excited characteristic modes before and after the void nucleation
For 360 atoms in the system, all 1080 modes are obtained using SVD. The variation of amplitude of modes excited in the system uniformly deformed at $5 \times 10^9$ s$^{-1}$ strain-rate before the void nucleation and after the first void nucleation is shown in figure 1 (a) and figure 1 (b), respectively.

![Figure 1](image1.png)

**Figure 1.** Amplitude of modes (singular values 'S') as a function of mode number (a) before the nucleation of a void (b) after the nucleation of a first void

4.2. Frequency Spectrum before and after the void nucleation
The comparison of frequency spectrum for first and third modes before and after the nucleation of first void is shown in figure 2 (a) and figure 2 (b), respectively. It is seen in figure 2 (b) that a shift in the frequency occurs after the nucleation of a void. In addition to this, some new frequencies also appear after the first void nucleation. The creation of new frequencies and a shift in frequencies are the signature of the nucleation of a void.

![Figure 2](image2.png)

**Figure 2.** Frequency spectrum of (a) mode 1 (b) mode 3

4.3. Temporal variation after the void nucleation
The temporal variation of the first strong mode after the first void nucleation is shown in figure 3. A sudden growth in the amplitude of the mode (figure 3) refers to the nucleation of a void in the system.

4.4. Spatial variation before and after the void nucleation
The spatial variation of first four modes excited in the system before and after the first void nucleation is shown in figure 4 (a) and figure 4 (b), respectively. The first strong mode before and after the void nucleation corresponds to the wavelength of $\lambda$. Other weak modes correspond to the wavelengths of $3\lambda/2$ and $5\lambda/2$. Note that hierarchy of the modes has been changed after the nucleation of a first void.

![Figure 4](image4.png)
5. Conclusions
We have performed uniform triaxial deformation of single crystal copper at $5 \times 10^9$/s strain-rate and data is analysed using singular value decomposition (SVD) technique. We find that after the nucleation of first void

- there is a shift in the frequencies of modes
- new frequencies are created
- strong modes correspond to the wavelength of $\lambda$, $3\lambda/2$ and $5\lambda/2$
- hierarchy of modes changes after the void nucleation

In future work, we plan to quantify the linkage between the change in mode behaviour (before and after void nucleation) and the nucleation process itself.

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