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DATABASE-ACCELERATED LOCAL QUASICONTINUUM METHOD BASED ON FIRST-PRINCIPLES DENSITY-FUNCTIONAL THEORY

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ABSTRACT

We proposed a new quasicontinuum finite-element method (FEM) analysis based on a numerical stress-strain database to calculate the non-linear large elastic deformation for single crystals. The database is constructed during finite-element analysis on-the-fly based on the first-principles density functional theory (DFT) calculations, which are able to obtain high-precision stress without any empirical parameters even under finite strained conditions. The database significantly improves the total computational efficiency without loss of accuracy. We also carried out parallel-computational method for the database construction process to realize further improvement of computational efficiency. The effectiveness of the proposed method is demonstrated through numerical simulation for several deformation tests of aluminum and diamond single crystals. We used VASP [1,2] and ABAQUS [3] for DFT and FEM analysis, respectively. Once the stress-strain database is constructed, total computational cost of DFT-based FEM analysis is reduced by 99% and above. The computational cost of database construction linealy decreases with incleasing number of processors.

Figure 1 shows stress-strain relation under $(111) < 11\bar{2} >$ shear deformation of a diamond crystal. Our quasicontinuum FEM analysis results are in good agreement with direct DFT analysis. Thus, our method has potential to estimate nonlinear elastic behavior and ideal strength of crystal under various external stress conditions.

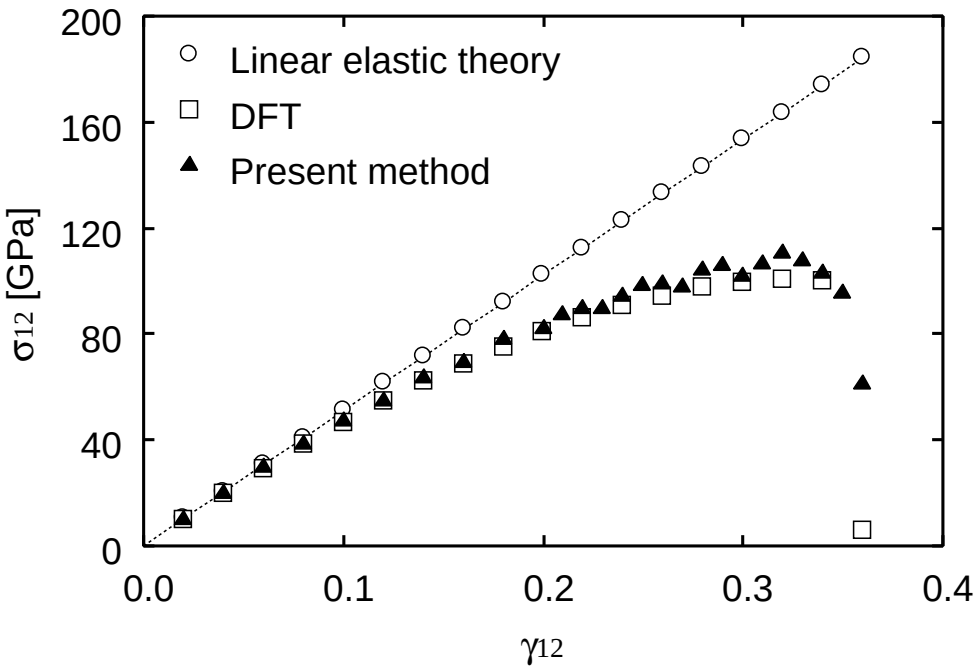

Figure 1: Stress-strain relation under shear deformation of a diamond crystal. Triangles and squares represent the data obtained from the present method and density-functional-theory (DFT) calculations, respectively. For comparison, the data from the linear elastic theory are indicated as circles.

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