Electronic and Atomistic Simulations on the Irradiation Induced Property Changes and Fracture in Materials

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Electronic and atomistic simulations have been performed to study the fundamental mechanical properties of metals with reference to irradiation, ductile-to-brittle transition, and fracture. For the electronic simulations, the VASP (Vienna ab-initio simulation package) code has been tuned on the Earth Simulator and its performance has been measured. The purpose of this simulation is to determine the Peierls stress of a screw dislocation in BCC Mo, whose core structures have not yet been clearly determined, and, finally, to understand the hydrogen embrittlement mechanism. For the atomistic simulations, the molecular dynamics code has been developed to introduce the layered link cell method to accelerate the vector calculations for the large scale simulations on the Earth Simulator. The purpose of this simulation is to understand the crack-tip microstructures in the fracture process and its interaction processes with the irradiation induced defects and grain boundaries.

Keywords: ab-initio simulation, dislocation, Peierls stress, molecular dynamics, fracture

1. INTRODUCTION

The detailed structure of electronic and atomistic bonding states of materials are required to understand fundamental mechanical properties of nuclear materials, in particular, embrittlement and fracture due to irradiation. Hydrogen embrittlement in BCC metals and development of microstructures near the crack-tip in the fracture process are the important applications in this field.

For the electronic simulations, the density functional theory (DFT) is the most dependable method to determine the core structure of a dislocation. We have tuned the VASP (Vienna ab-initio simulation package) code on the Earth Simulator to perform a large-scale simulation and measured its performance. The purpose of this simulation is to determine the Peierls stress of a screw dislocation in BCC Mo, whose core structures have not yet been clearly determined, and, finally, to understand the hydrogen embrittlement mechanism for iron.

For the atomistic simulations, we have developed the molecular dynamics code to introduce the layered link cell method to accelerate the vector calculations for the large scale simulations on the Earth Simulator. The purpose of this simulation is to understand the crack-tip microstructures in the fracture process and its interaction processes with the irradiation induced defects and grain boundaries.

2. COMPUTATIONAL METHOD AND RESULTS

2.1. Density Functional Simulation on the Dislocation Core Structure

For the final assessment of the hydrogen embrittlement mechanism in BCC metals, it is firstly important to determine the Peierls stress of BCC metals. BCC metals, in general, become brittle at low temperatures, and the exact core structure of a screw dislocation of the Burgers vector of a/2<111> is needed to understand the flow and fracture mechanism. However, we have not yet obtained the definitive answer for this problem. Experiments are still difficult, and the results of computational approaches depend on interatomic potential and boundary condition. The value of the Peierls potential depends on simulation methods, ranging from 2 GPa to 4 GPa. There are two proposed core structures of a screw dislocation as a result of the calculations using the empirical potentials, tight binding method, and the density functional theory. The density functional theory is the most dependable method, but its kpoint convergence is still unclear. In order to find a definitive solution to this problem, the following three points must be considered. First, we need to have a well-defined boundary condition for this problem. This has been already checked and the system consisting of 231 atom supercell, as shown in Fig. 1, is found to be accurate for this

purpose. Secondly, we need to evaluate the accurate total energy expression for this system. The VASP (Vienna ab-initio simulation package) code, which implements the density functional theory with the ultrasoft pseudopotential, suits this purpose. Thirdly, computational conditions have to be clarified by the careful error estimation, including plane wave and kpoint convergence checks.

The MPI parallel code of the VASP has been tuned to the Earth Simulator. Mainly, the one-dimensional FFT routine has been replaced by the numerical library ASL/ES. It is found that the tuning for vector processing by compiler optimization on the Earth Simulator can result in the inconsistency with the installed copy of the linear equation solver library LAPACK. This has been remedied and the VASP code has been debugged for the implementation of the code to the Earth Simulator. The vector operation ratio has been measured using up to the 64 processors, and the ratio of approximately 99% has been achieved, as shown in Table 1. The parallel three dimensional FFT and the communication part of the program will be tuned for the next term.

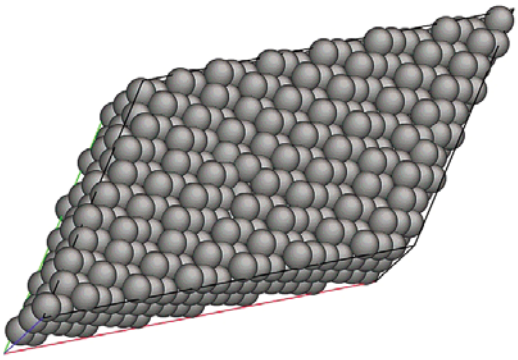

Fig. 1 The BCC Mo supercell consisting of 231 atoms

The relaxation of the BCC Mo perfect lattice structure has been performed by checking the energy convergence by increasing the kpoints. Phonon dispersion curve of BCC Mo 250 atoms using $6 \times 6 \times 6$ kpoints is obtained in Fig. 2, and the detailed structure near the H point has been reproduced compared with the experimental data.

2.2. Molecular dynamics simulation for the fracture of polycrystalline metal

The purpose of the atomistic simulation is to study the mechanistic details of crack-tip microstructures in the frac-

Table 1 Vector performance of the VASP code on the Earth Simulator

Average	16 processes	32 processes	64 processe
Real Time (sec)	709.435	441.026	342.213
MFLOPS	4715.369	4040.298	3242.151
Average Vector Length	226.940	218.488	197.904
Vector Operation Ratio (%)	99.081	98.803	98.348

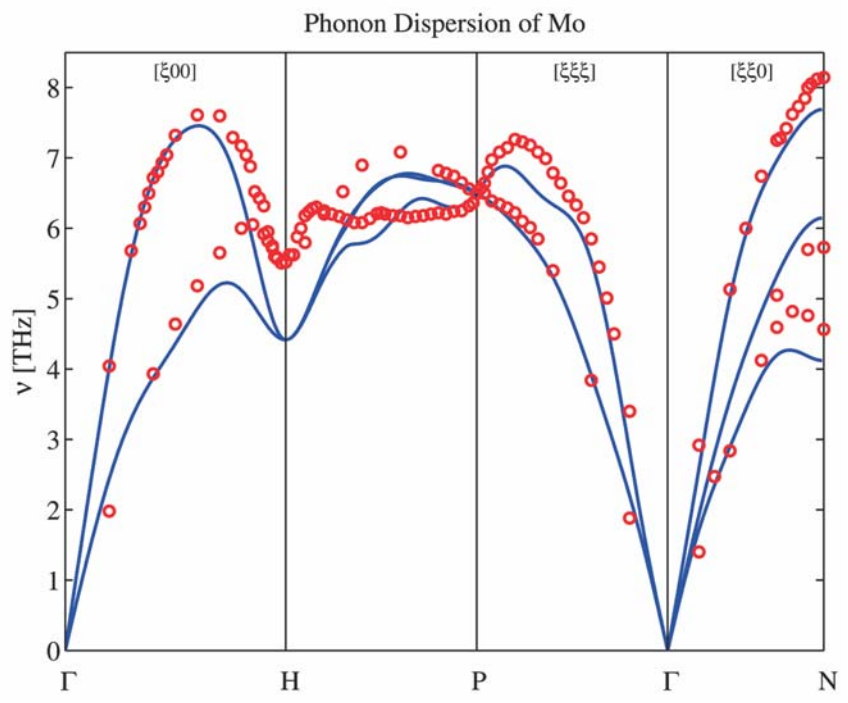

Fig. 2 Phonon dispersion curve of BCC Mo 250 atoms with $6 \times 6 \times 6$ kpoints.

ture process and its interaction processes with the irradiation induced defects and grain boundaries, and finally to understand the brittle-to-ductile transition mechanisms for the three dimensional grain boundary fracture process. Since the algorithm of short-range empirical potential molecular dynamics method is suited for the massively scalar supercomputers, the layered link method [1], in which the vector length is proportional to the number of atoms, is adopted for the implementation on the Earth Simulator. The domain decomposition method, which achieves a good scalability by communicating between contacting neighbor processors, is adopted for the parallelization of the program. Since the parallelization code is localized, the tuning of parallel processing is done independently of that of vector processing. The embedded atom method (EAM) potential is introduced in the program for the realistic modeling of the fcc metals. The program is ready for the performance test and simulation on the Earth Simulator.

3. SUMMARY

The VASP (Vienna ab-initio simulation package) code has been tuned on the Earth Simulator and its performance has been measured. The kpoints convergence check is in progress, and the accurate phonon dispersion curve for BCC Mo metal is obtained.

The molecular dynamics code has been developed to introduce the layered link cell method to accelerate the vector calculations for the large scale simulations on the Earth Simulator. The program is parallelized for the implementation on the Earth Simulator.

Reference

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