Discussion of J-integral around a moving dislocation in discrete system

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1. Introduction

J-integral has been widely applied to characterize fracture properties of both brittle and ductile materials. According to continuum elasticity, the J-integral around a defect has a physical meaning as a configuration force acting on the defect [1]. As a result, the J-integral is equal to Peach-Koehler (PK) force when it is calculated around a stationary dislocation. Especially, the J –integral is given by an integral form and it shows path-independent behavior by the conservation theorems.

According to continuum elasticity, the same result is deduced when it is calculated around an uniformly moving dislocation without acceleration as long as the system is continuous [2]. In this work, however, we theoretically prove that the J-integral is no longer equal to PK force when the dislocation moves in discrete system and support our theoretical result by molecular dynamics simulation.

2. Theory

For an arbitrary closed contour path Γ, the static J-integral along i-direction is defined by Eq. (1).

$$J_i = \oint_{\Gamma} (W n_i - T_j u_{j,i})\, d\Gamma \qquad (1)$$

where W is strain energy density, T is traction, u is displacement and n is normal vector to Γ. According to the continuum theory, the J-integral is equal to Peach-Koehler (PK) force as

$$J^{cont} = F^{PK} = \sigma_{app} b\,. \qquad (2)$$

where σ_{app} is applied shear stress and b is Burgers vector for a stationary dislocation. And it is equal for a dislocation that uniformly move without acceleration. However, in this work, we proved that Eq. (2) should be changed to Eq. (3) when the dislocation moves in discrete system.

$$J^{disc} = \sigma_{app} b + F_{drag}(w, R)\,. \qquad (3)$$

Here, the second term of Eq. (3) is an additional force caused by a drag effect around the dislocation core and it makes J^{disc} be smaller than J^{cont} [3]. In other words, F_{drag} acts on the dislocation opposite to the applied force. In particular, the drag force depends on the dislocation core width w, and integration size, R.

3. Molecular dynamics simulation method

First, we construct neat a nickel nanowire that consists of 900, 60, 6 atoms along x, y and z directions, respectively. The each axis is parallel to $[\bar{1}\,\bar{1}\,2]$, $[111]$, and $[\bar{1}10]$, respectively. To calculate interaction between nickel atoms, Angleo EAM [5] interatomic potential was used. A periodic boundary condition was applied along z direction but atoms were allowed to be relaxed along both x and y directions. Then, system's potential energy was minimized by using conjugation gradient scheme at 0 K.

After the energy minimization, a single screw dislocation was inserted by applying elastic displacement field to every atom [5]. Here, both the dislocation line and Burgers vector were parallel to the z direction and the Burgers vector was defined as $\mathbf{b} = 1/2[\bar{1}10]$. However, the Burgers vector was divided into two partial dislocations in face-centered cubic crystals to lower the system's energy. As a result, an extended dislocation, which consists of two partial dislocations and a stacking fault between them, was formed as shown in Fig. 1. The Burgers vector of the leading partial was $\mathbf{b}_l = 1/6[\bar{2}11]$ and it of the trailing partial was $\mathbf{b}_t = 1/6[\bar{1}\,2\,\bar{1}]$. After the dissociation of a perfect dislocation, the energy of system was minimized again.

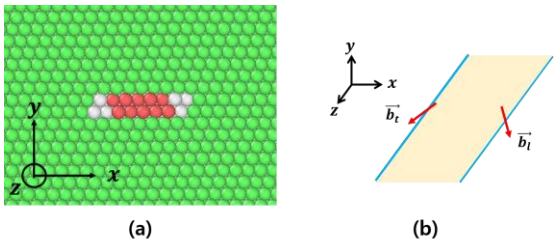

Fig. 1. (a) Equilibrium dislocation core in nickel. Color represents a common neighbor analysis. (b) Schematic of an extended dislocation. Partial dislocations are represented by blue lines. And the shaded region represents a stacking fault between them.

Then, constant stress was applied by pushing top and bottom y surfaces in opposite direction. For every 1 fs, the atomic position was updated by NPT ensemble with maintaining 0 K and $\sigma_{11} = \sigma_{22} = \sigma_{33} = 0$. As a result, the dislocation began to move and finally reached to steady state.

4. Result

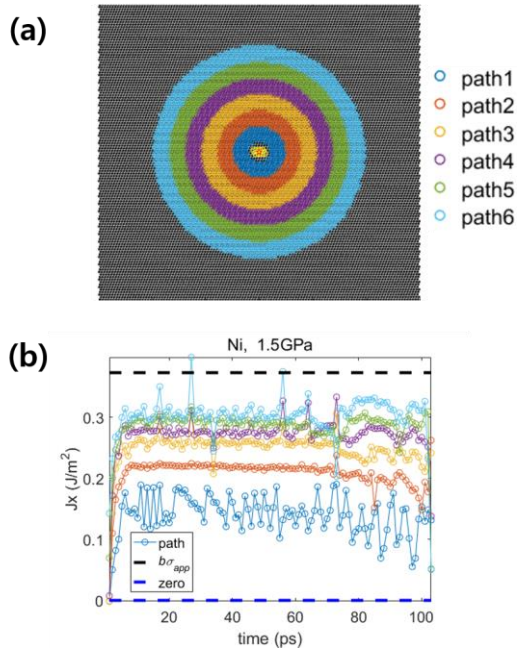

Fig 2. (a) Definition of contour paths to calculate the J-integral (b) The J-integral calculation during the motion of dislocation under $\sigma_{app} = 1.5 GPa$. The dotted line represents PK force defined by Eq. (2).

We defined various circular paths to calculate J-integral as shown in Fig. 2(a). As a result, we observed that the J-integral values were always lower than the PK force and increased with increasing the path size as shown in Fig. 2(b). Then, we compared the deviations between them with F_{drag} derived by our theory. This is shown in Fig. 3. From Fig. 3, there were good agreements between our theoretical prediction and the simulation results.

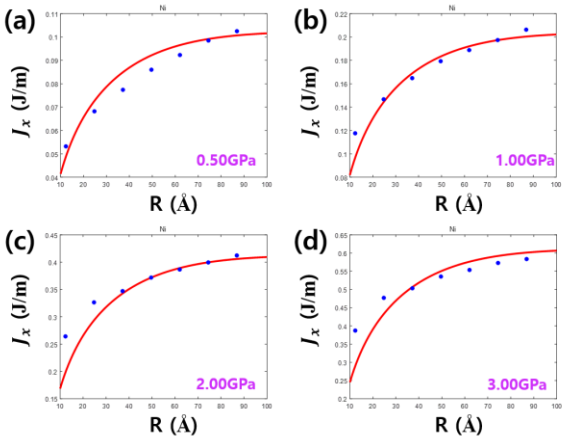

Fig. 3. Relationship between the J-integral and integration radius for the moving dislocation under various stress. Red line represents F_{drag} obtained by our theory and blue dots represent MD simulation results. Each figure corresponds to when (a) $\sigma_{app} = 0.50\,\text{GPa}$, (b) $\sigma_{app} = 1.00\,\text{GPa}$, (c) $\sigma_{app} = 2.00\,\text{GPa}$, and (d) $\sigma_{app} = 3.00\,\text{GPa}$

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References

[1] J. D. Eshelby, The force on an elastic singularity, *Philosophical Transactions of the Royal Society A*, 244 (1951) 87-112.
[2] A. N. Stroh, Force on moving dislocation, *Physical Review*, 128 (1962) 55-61.
[3] S. Kim, D. T. Ho, K. Kang, S. Y. Kim, Phonon scattering during dislocation motion inducing stress-drop in cubic metals, *Acta Materialia*, 115 (2016) 143-154.
[4] J. E. Angelo, N. R. Moody, M. I. Baskes, Trapping of hydrogen to lattice defects in nickel, *Modelling and Simulation in Materials Sciecne and Engineering*, 3 (1995) 289-307.
[5] J. P. Hirth, J. Lothe, *Theory of dislocations*, Krieger, Florida, 60-78.