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Application of continuous CVM to extended lattice defects in materials

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A new formulation of the CVM which allows atomic displacement from lattice points is used to calculate the atomic configurations of the extended lattice defects (cleaved surface and a crack) at finite temperatures. We formulate continuous atomic displacements around lattice points using the pair approximation of the CVM, and study the temperature dependence of the atomic configurations and thermodynamical properties of the extended lattice defects.

1. INTRODUCTION

So far, most of the atomistic simulation studies of the lattice defects have been performed assuming the absolute zero temperature. However, the lattice defect properties of materials often depend strongly on the temperature. For instance, it is known that fracture behavior of materials depends strongly on the materials parameters, such as temperature, strain rate, and external chemical environment [1-4]. In the present study, we focus our attention on the thermal (temperature) effects on the fracture behavior of a simple solid. In the exsisting CVM formulations, atoms are placed on lattice points. We introduce a new formulation, continuous treatment of CVM in which atoms can be displaced from a lattice point [5]. Using the continuous CVM, we investigate the atomic bond breaking process in the crack-tip region, of 2D square lattice.

2. PRINCIPLE OF CALCULATION

The easiest approach to atomic phenomena at crack tips is to consider an infinite lattice of atoms in which a crack is formed by slitting the bonds between rows in two dimensions. A force is then applied to the center atom pair which is required to hold the cracked atoms apart. For zero temperature calculations, we use a lattice Green's function method for the atomistic

displacements of the crack. The atomic geometry of a crack in two-dimensional (2D) square lattice is shown in Fig.1. For simplicity, we consider the small cracks with one and three bonds broken.

When the external force F=0, the system is homogeneous and reduces to the previous treatments [5] for the perfect lattice. When the external force F is applied, first we have to identify a lattice point location. But the basic equations remain practically the same as long as the external force F is not large, except the pair PQ in Fig.1. We need a work done by external force F on the pair and include it as follows.

$$g(\mathbf{r_P},\mathbf{r_Q})=\exp(\beta\lambda_{PQ}/2)\exp[-\beta\varepsilon(\mathbf{r_P},\mathbf{r_Q})+ \beta F(y_P-y_Q)](f(\mathbf{r_P})\, f(\mathbf{r_Q}))^{\frac{3}{4}}\Gamma_{corr} \quad , \quad (1)$$

where y_P is the y axis of P. Since $(y_P-y_Q)F$ is the work done by F on the pair, it is the increase in the energy of the pair. When the external force F is positive and is pulling P and Q away, $(y_P-y_Q)>0$ is more plausible than $(y_P-y_Q)<0$, indicating the sign + in front of the force term. The above mentioned characteristics are the basic heuristic description of the equations we work with.

The free energy is composed of four terms describing internal energy, configurational enthropy, normalization condition of pair distribution functions and Lagrange multipliers for the symmetry constraint conditions. We minimize the free energy Ψ of the system with respect to the pair distribution functions g_x and g_y, in order to obtain the thermodynamically equilibrium solutions.

3. RESULTS AND DISCUSSIONS

The atomistic studies on cracks in crystalline materials at absolute zero temperature have been performed by using the lattice Green's function method [1,2]. The atomic displacements due to the external forces are calculated accurately (exactly) by using the lattice theory: The lattice trapping of the crack and crack stability relations have been calculated and the fundamental aspects of fracture behavior at absolute zero temperature have been clarified.

In order to understand the fundamental properties of the cracks at finite temperatures, entropy terms must be added to the energetics. This type of entropy effect (lattice vibration effect) can be taken into account efficiently within the present continuous CVM treatment. In the present calculation, we introduce small cracks in the 2D square lattice, as shown in Fig.1: Figures 1 (a) and 1(b) are schematic drawings for the smallest and small crack with three broken bonds, respectively.

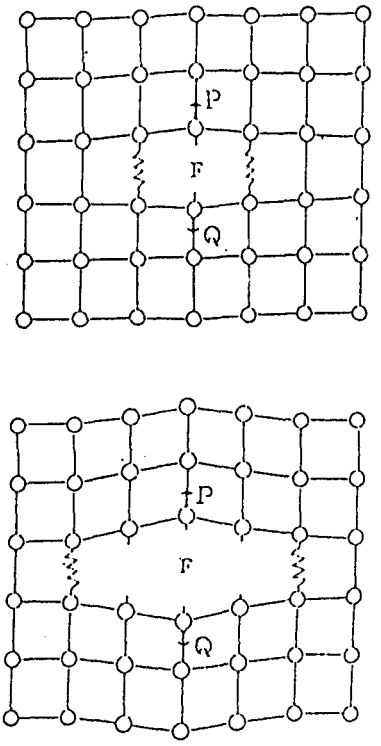

Fig.1 Atomic geometries of small cracks.

We calculate the atomic displacements around the cracks as a function of temperature and external dipole force F. Figure 2 shows the point distribution function at the central atom site in the crack. In Fig.3, we present the atomic displacements u_0 and u_1, by solid lines, as a function of the external load F at kT/ε_0 = 0.6. In Fig.3, we also present, by dot-dashed curves, the atomic displacements u_0 and u_1 of the lower temperature kT/ε_0 = 0.4, where ε_0 denotes the pair interaction energy between nearest-neighbour atoms in the perfect lattice at absolute zero temperature. When one uses Lennard-Jones potential, ε_0 is simply the energy parameter

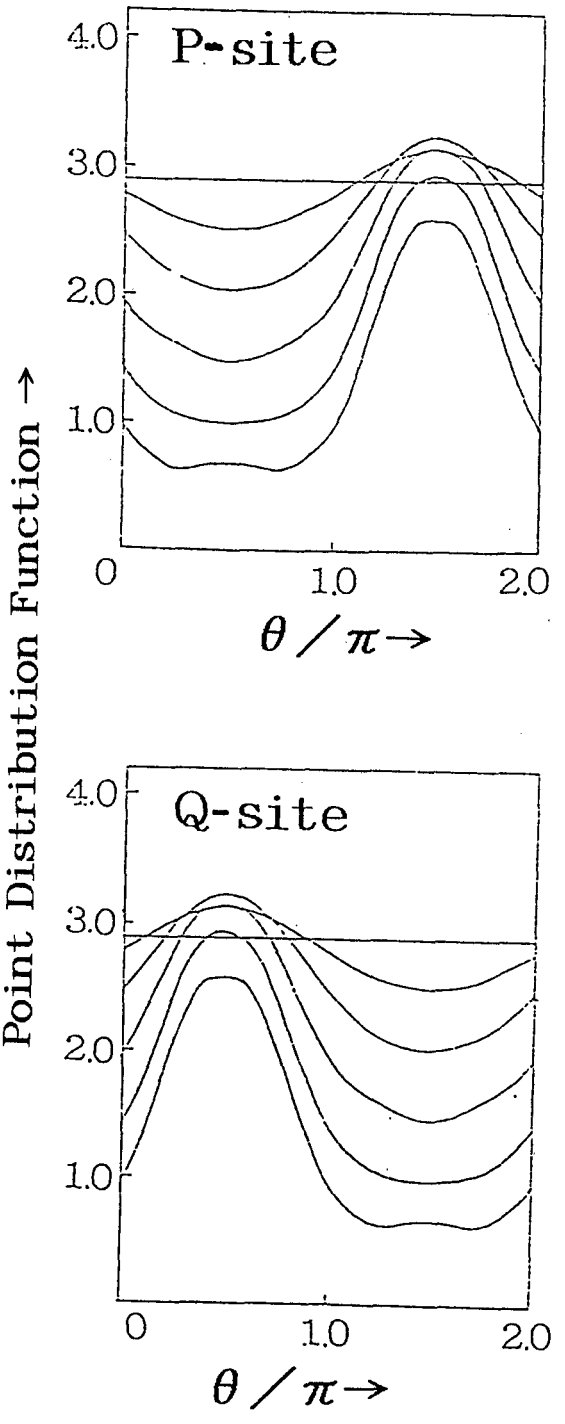

Fig.2 Point distribution function $f(\rho,\theta)$ at the central site of the smallest crack.

of the potential [5]. Atomic displacement u_0 at higher temperature becomes larger compared to that at lower temperature. On the other hand, we have found that the atomic displacement u_1 at higher temperature becomes smaller compared to that at lower temperature. This indicates that stress intensity factor K_I at higher temperature becomes larger and the material becomes more ductile compared to those of lower temperature.

Finally, it is noted that the present continuous CVM can also be applied to study the dislocation emission criteria and estimate crack stability relation at finite temperatures.

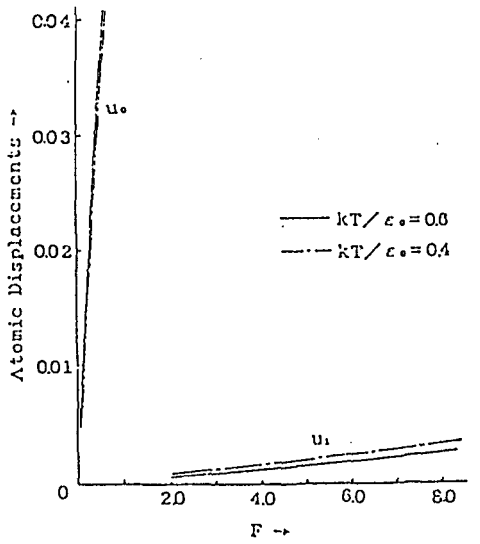

Fig.3 Atomic displacements u_0 and u_1 at temperature kT/ε_0 =0.4 and 0.6.

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