Plastic Deformation of Nano-Size Copper Specimens Title

Masao Doyama, Yoshiaki Kogure, and Tadatoshi Nozaki
Department of Environmental Science, Teikyo University of Science and Technology
Uenohara, Yamanashi, Japan

ABSTRACT

Copper nano-size specimens with and without cracks are pulled, compressed, and bent using molecular dynamics with an embedded atom potential. A crystal contains several thousands atoms. Single crystals are rectangular parallelepipeds. Dislocations created were always partial dislocations in copper. Nano Lang X-ray photographs and Laue X-ray photographs are also simulated using the deformed atomic positions obtained by molecular dynamics. When there are atomic steps on the surfaces of specimens, partial dislocations started at the steps. These simulation results can be applied for understanding the mechanism of plastic deformation of nano-materials with scratches or surface corrosion on the surfaces.

KEY WORDS: Plastic deformation; copper; single crystals; partial dislocations; tensile deformation; compression.

INTRODUCTION

Plastic deformation of small nano-size crystals is becoming important not only in science but also in technology fields. The precision processing of metals requires the knowledge even on atomic scale. The purpose of this study is to understand plastic deformation of metals on atomic scale. In this paper, plastic deformation of copper single crystals has been studied by computer simulation using molecular dynamic method with an embedded atom potential. For simplicity, copper single crystals have been chosen to study, because copper has face centered cubic crystal structure and ductility even at low temperatures.

INTER-ATOMIC POTENTIAL

In metals, the conduction electron transfers from one atom to another and the interaction cannot be represented by pairwise potentials. The interaction between the i-th atom and the j-th atom depends not only on the distance between them but also on the positions of other atoms around them. Copper was chosen as an example of a face centered cubic lattice. The n-body embedded function proposed by us [Doyama and Kogure, 1999] was used. The total energy of a sample is given by

\[ E_{\text{total}} = \sum_i E_i \]  
\[ E_i = F (\rho_i) + (1/2) \sum_{j \neq i} \phi (r_{ij}) \]  
\[ r_{ij} = | r_i - r_j | \]  
\[ F (\rho_i) = D \sum_j \rho_j \ln (\rho_i) \]  
\[ \rho_i = \sum_j f (r_{ij}) \]

We assumed [Doyama and Kogure, 1999]

\[ \phi (r_{ij}) = a_1 (r_{ij} - r_0)^2 \exp(-c_1 r_{ij}) \]  
\[ f (r_{ij}) = a_2 (r_{ij})^{c_2} \exp(-c_3 r_{ij}) \]  
\[ \phi (r_{ij}) \text{ and } f (r_{ij}) \text{ are smoothly truncated at } \phi (r_{ij}) \text{ and } f (r_{ij}) \text{, respectively. } r_{c1} \text{ was chosen to be } 1.65d, \text{ where } d \text{ is the nearest neighbor distance. } r_{c2} \text{ was chosen to be } 1.95d. \text{ The potential functions described in Eqs. 1 ~ 7 contain five parameters. } a_1 = 8289.46000/d^2, a_2 = 0.0183251035/d^2, c_1 = 10.727291/d, c_2 = 0.319759370/d \text{, and } D = 13.0792125 \text{ for copper. In these cases } d \text{ is the nearest neighbor distance in cm, and the energies are represented in erg. These parameters are determined to reproduce the Born stability, cohesive energy, elastic constants } c_{11}, c_{12}, \text{ and } c_{44}, \text{ the formation energy of a vacancy, and stacking fault energy.}

SPECIMENS

Specimen S shown in Fig. 1(a) is a rectangular parallelepiped and the surfaces are (001), (00-1), (01-1), (011), and (01-1). X-axis, Y-axis, and Z-axis are taken to be [00-1], [01-1], and [011], respectively.

![Fig. 1. Specimens](a)