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Quantitative measurement of deformation field around low-angle grain boundaries by electron microscopy

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Abstract

The strain field of low-angle grain boundaries in gold was experimentally investigated. The grain boundaries consist of the arrangement of discrete dislocations. High-resolution transmission electron microscopy (HRTEM) and geometric phase analysis (GPA) were employed to map the strain field of grain boundaries. The numerical moiré method was used to visualize the dislocations. The strain components ε_{xx}, ε_{yy}, ε_{xy} and rigid rotation ω_{xy} were mapped. The dislocation core regions are convergence regions of strain. The largest values of strain occur in the immediate dislocation core region. The strain field around an edge dislocation was compared with Peierls–Nabarro dislocation model. The comparison result has demonstrated that the Peierls–Nabarro model can describe the strain field around edge dislocation.

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1. Introduction

The properties of materials are strongly influenced by the presence of grain boundaries. Low-angle grain boundaries consist of arrays of discrete dislocations that separate two crystals of slightly different orientation. The dislocation model for low-angle grain boundaries was firstly proposed by Taylor [1], and further developed by Read and Shockley [2] to predict dislocation density from macroscopic boundary geometry. Read and Shockley used their model to calculate boundary energy based on the summed elastic energy of the individual dislocations. The dislocation model is still the basis for understanding low-angle grain boundaries. Experimental measurements of strain field of low-angle grain boundary structures will help to understand how it influences the material's properties.

Moiré interferometry has been used to measure deformation to 300 nm [3]. Electron beam moiré has been used to measure deformation to 100 nm [4]. Nano-moiré method has been used to measure deformation to 0.1 nm [5,6]. The scanning moiré method [7] is developed and applied to the deformation measurement at the nanometer scale. The digital nano-moiré method [8] is proposed and the displacement measurement sensitivity can reach the pitch of the lattice of a single crystal (sub-nanometer level). Geometric phase analysis (GPA) [9] and numerical moiré [10], two recently developed techniques that are sensitive to small displacements of lattice fringes in high-resolution transmission electron microscopy (HRTEM) images. They have been applied to a wide variety of systems such as nano-structured Cu–Ag materials [10], quantum dots [11], nano-wires [12], Al/Si nano-cluster [13]. The accuracy of the GPA has been demonstrated that could be measured to 0.003 nm [14]. In this article, we have analyzed the structure and deformation field of low-angle grain boundaries using HRTEM and GPA method. Strain components ε_{xx}, ε_{yy}, ε_{xy} and rigid rotation

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ω_{xy} around low-angle grain boundaries were mapped. And the strain field around an edge dislocation was compared with Peierls–Nabarro dislocation model [15,16].

2. Experimental methods

2.1. Geometric phase analysis

An HRTEM image formed at a zone axis of a crystal can be considered as a set of interference fringes corresponding to the atomic planes of the specimen. GPA analyzes these interference fringes individually to extract the information concerning displacement. In particular, the technique measures the displacement of lattice fringes with respect to a perfect lattice (for example, provided by a region of undistorted substrate). The method is based on the calculation the local Fourier components of lattice fringes. The phase of these local Fourier components, or geometric phase $P_g(\boldsymbol{r})$, is directly related to the component of the displacement field, $\boldsymbol{u}(\boldsymbol{r})$, in the direction of the reciprocal lattice vector g:

$$P_g(\boldsymbol{r}) = -2\pi \boldsymbol{g} \cdot \boldsymbol{u}(\boldsymbol{r}). \quad (1)$$

It is assumed that the displacement field is constant along the propagation direction through the foil or that if there are small variations, they are averaged out. In the latter case, the displacement field is the projected displacement field averaged over the foil thickness. And by measuring two phase images, $P_{g1}(\boldsymbol{r})$ and $P_{g2}(\boldsymbol{r})$, the two-dimensional displacement field, can be determined:

$$\boldsymbol{u}(\boldsymbol{r}) = -\frac{1}{2\pi}[P_{g1}(\boldsymbol{r})\boldsymbol{a}_1 + P_{g2}(\boldsymbol{r})\boldsymbol{a}_2]. \quad (2)$$

Here $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the basis vectors for the lattice in real space corresponding to the reciprocal lattice defined by $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$. Eq. (2) in matrix form:

$$\begin{pmatrix} u_x \\ u_y \end{pmatrix} = -\frac{1}{2\pi}\begin{pmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{pmatrix}\begin{pmatrix} P_{g1} \\ P_{g2} \end{pmatrix}. \quad (3)$$

Plane strain can be written as

$$\begin{cases} \varepsilon_{xx} = \dfrac{\partial u_x}{\partial x} \\ \varepsilon_{yy} = \dfrac{\partial u_y}{\partial y} \\ \varepsilon_{xy} = \dfrac{1}{2}\left(\dfrac{\partial u_x}{\partial y} + \dfrac{\partial u_y}{\partial x}\right) \end{cases} \quad (4)$$

and rigid rotation can be written as

$$\omega_{xy} = \frac{1}{2}\left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}\right). \quad (5)$$

2.2. Electron microscopy

HRTEM sample consists of an ultra-thin layer of gold grown epitaxially into single crystals along the [0 0 1] direction. HRTEM experiments were performed on the JEOL 2010 transmission electron microscope at 200 kV (spherical aberration = 1.0 mm, point resolution = 0.194 nm). Images were recorded on a Gatan 1024 × 1024 slow scan CCD camera and processed using the software GPA Phase [17], developed in the Gatan Digital Micrograph environment.

3. Results and discussion

Fig. 1 shows a transmission electron microscopy image of low-angle grain boundaries in gold. The boxed region is part of the grain boundaries. Its HRTEM image is shown in Fig. 2(a). Fig. 2(b) shows Fourier transform of the HRTEM image. Phase images were calculated for the two sets of {2 0 0} lattice fringes using Gaussian masks, and are shown in Fig. 2(c, d). To visualize this arrangement, two numerical moiré images have been calculated by using a magnification factor of three. The result is shown in Fig. 2(e, f). The moiré pattern acts as a lens which magnifies not only the lattice spacing but also the deformation and rotation. It can be seen that low-angle grain boundaries consist of the arrangement of discrete dislocations. The deformation occurred in the dislocation of grain boundaries.

Taking x-axis parallel to [0 1 0] and y-axis parallel to [$\bar{1}$ 0 0], the strain fields, ε_{xx}, ε_{yy}, ε_{xy}, calculated from Eqs. (3) and (4), are shown in Figs. 3(a–c). There are some convergence regions of strain. The largest values of strain occur in the immediate dislocation core region. Fig. 3(d) shows the rigid rotation map ω_{xy}. The in-plane rotation between left grain and right grain is about 2°.

The boxed region in Fig. 3(a) is clockwise rotated 29° and magnified in Fig. 4(a). This is an edge dislocation,

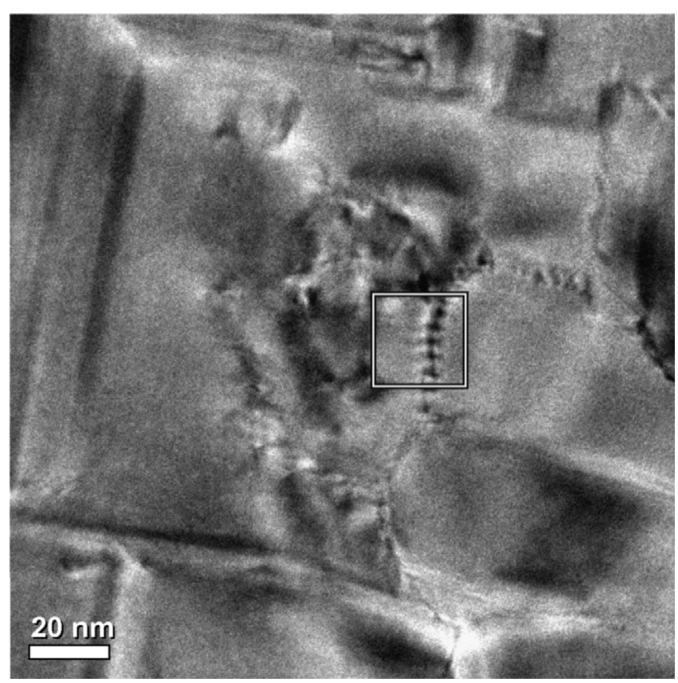

Fig. 1. Transmission electron microscope image of grain boundaries.