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Investigation of continuous deformation behavior around initial yield point of single crystal copper by using micro scale torsion test

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ABSTRACT

Micro scale torsion test method was developed to investigate continuous deformation behavior around initial yield point of copper single crystal structure. Continuous load–displacement curve was obtained by torsion test because dislocation burst phenomenon was suppressed by stress gradient and torsion stress direction which parallel to the specimen surface. In case that new constitutive law was applied to the simulation, crystal plasticity parameter of copper could be evaluated by parameter fitting which using load–displacement curve of experiment and simulation.

1. Introduction

Continuous deformation behavior around initial yield point of micro scale single crystal structure was investigated in this study. In recent years, deformation of micro scale single crystal was frequently investigated by indentation [1–5], bending test [6], compression of micro pillar [7–10], and tensile test [8,9,11–13]. In case of these test, it is well known that uncontinuous deformation behavior was shown under examination because of the unsaturated slip deformation due to penetration of large amount of dislocation of single slip system to specimen surface. This unsaturated large slip deformation behavior is called dislocation burst (strain burst, deformation burst et al.) phenomenon [7–12]. In case of conventional test such as tensile and compression test, stress field of these tests are homogenous. Then it is considered that one of the causes of dislocation burst is yielding of all cross section of specimen at the same time. In other words, in case that stress field of specimen is not homogenous, it is assumed that continuous deformation behavior around initial yielding point without dislocation burst can be obtained. Moreover, by using simulation including the effect of crystal plasticity, crystal plasticity as material property of micro scale single crystal also can be evaluated. If these results are obtained, characteristic of the dislocation burst can be evaluated. However, continuous deformation behavior of micro scale crystal structure cannot be obtained by conventional technique. Therefore in this study, new type small scale torsion test method to obtain continuous deformation behavior around initial yield point was developed by using copper single crystal specimen. In torsion test, it is considered that dislocation burst is suppressed because slip direction of torsion test is not facing to the specimen surface and torsion load after surface yielding was kept by elastic region at inside of specimen due to stress gradient.

In this study, development of micro torsion test method and evaluation of crystal plasticity parameter of copper single crystal were conducted by comparing result of experiment and numerical simulation which is including the effect of crystal plasticity. Program of crystal plasticity constitutive law of single crystals in a continuum modeling which using the user subroutine UMAT of the commercial finite element code ABAQUS has been developed by Huang [14] and which modified by Kysar [15], and which theory

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of crystal plasticity was developed by Peirce [16], Hutchinson [17], et al. This program was used to simulate crystal plasticity in this study.

2. Experimental procedure

Specimen fabrication and experiment were conducted by testing system which is composed of a nano-indenter system and a focused ion beam (FIB) gun attached to scanning electron microscopy (SEM) system [18]. Design of the specimen shape looks like semi-circular arc (with 2.5 μm radius, 1 μm width and thickness) of cantilever, and torsion load was applied by indentation load to out-of-plane direction at the end of cantilever. Single crystalline Cu torsion specimen was fabricated by FIB, which is made by Copper single crystal (M.T.I Corporation, 99.9999% purify). Fig. 1 (a) and (b) show SEM image of the micro torsion specimen which before and after experiment, respectively. For Fig. 1(a), torsion specimen was correctly fabricated by FIB. In Fig. 1(b), traces of large slip deformation thought cross section of specimen was not observed in specimen after torsion test. Crystal orientation of copper single crystal is explained by using axis of Fig. 1(a), integer index of Z angle is [23 10 4], and integer index of Y angle is [−25 52 10]. In the experiment, specimen was put on the specimen holder in SEM with nano indenter, and torsion test was conducted by using indenter with Berkovich tip. Test speed of indenter is 10 nm/s, and edge radius of Berkovich tip is about 130 nm.

3. Numerical simulation

Finite element method (FEM) model of torsion specimen was designed for actual specimen shape (Fig. 1(c)), and it was created by using the commercial FEM code ABAQUS 6.11-2. Brick element with 8 nodes was used, and number of elements are 11298. In this study, ABAQUS user subroutine program UMAT to incorporate Cu single crystal plasticity constitutive hardening laws which was written by Huang [14] was implemented. In this program, based on the Schmid's law, the slipping rate $\dot{\gamma}^{(\alpha)}$ of the αth slip system in the rate-dependent crystalline solid is determined by the corresponding resolved shear stress $\tau^{(\alpha)}$ which is as follows:

$$\dot{\gamma}^{(\alpha)} = \dot{a}\left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right)\left|\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right|^{n-1}, \tag{1}$$

where the constant $\dot{a}^{(\alpha)}$ is the reference strain rate on slip system α, $g^{(\alpha)}$ is the flow stress of that system, n is the rate sensitivity exponent which used for simple power law for polycrystalline creep. The strain hardening is determined by the evolution of the strengths $g^{(\alpha)}$ through the incremental relation:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}\dot{\gamma}^{(\beta)}, \tag{2}$$

where $h_{\alpha\beta}$ are the slip hardening moduli. $h_{\alpha\alpha}$ and $h_{\alpha\beta}$ are called self and latent hardening moduli, respectively. Hardening model which plastic deformation of each slip system was given by:

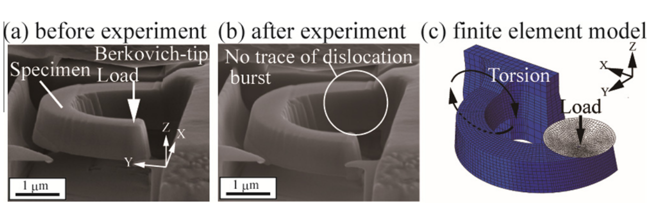

Fig. 1. Torsion test specimen. SEM image of torsion test specimen for in-site test and finite element model which imitation of actual torsion test. Torsion test was carried out by using Berkovich indenter. (a) SEM image of torsion specimen before test. (b) After torsion test. (c) Finite element model of torsion test.

$$h_{\alpha\alpha} = h(\gamma) = h_0 \,\mathrm{sech}^2\left|\frac{h_0\gamma}{\tau_s - \tau_0}\right|, \tag{3}$$

$$h_{\alpha\beta} = qh(\gamma) \quad (\alpha \neq \beta), \tag{4}$$

where γ is the shear strain, τ_s is the stage I stress, τ_0 is the yield stress which equals the initial value of flow stress $\tau(0)$, h_0 is the initial hardening modulus of the slip system, and q is a constant. Hardening law which was based on current value of flow stress of the single slip system as follows:

$$\tau(\gamma) = \tau_0 + (\tau_s - \tau_0)\tanh\left(\frac{h_0\gamma}{\tau_s - \tau_0}\right), \tag{5}$$

where $\tau(\gamma)$ is the current value of the flow stress in a single slip (shear stress). Material parameter of copper for the single crystal constitutive model excluding fitting parameters is shown in Table 1. Elastic constants are the same of bulk copper single crystal in case of micro structure [19]. Fitting parameters are h_0, τ_0, τ_s and q, and parameter fitting was conducted by using load–displacement curve of experiment and result of simulation. However, in case that conventional constitutive equation was used, parameter fitting was impossible. Therefore, new constitutive law was developed. For new constitutive law, flow stress shows sudden drop at initial yield point and after that general hardening behavior such as yield behavior of bulk BCC metal. New constitutive law is as follows:

$$\begin{aligned} &\tau(0) = \tau_x \\ &\tau(\gamma) = \tau_0 + (\tau_s - \tau_0)\tanh\left(\tfrac{h_0\gamma}{\tau_s - \tau_0}\right) \quad (\gamma > 0) \end{aligned} \tag{6}$$

where τ_x is initial value of flow stress. In this law, flow stress downs to τ_0 from τ_x when resolved shear stress reaches τ_x, and the rest is same as conventional constitutive law.

4. Result and discussion

Fig. 2 shows that applied load–displacement curve of actual torsion test. 2 specimens were used for testing. Difference of maximum load and gradient of elastic area between these results are probably due to deviation of accuracy of specimen shape and position of loading point. For the torsion test, almost continuous curve was obtained. Though these tiny load drops were observed, load drop is much smaller than that of conventional method due to dislocation burst [7–12] and points of tiny load drop are not initial yield point. Traces of dislocation burst phenomenon couldn't be observed at specimen surface in SEM image of after experiment (Fig. 3(b)) such as step at surface [7,12]. Then, it is assumed that dislocation burst was suppressed in torsion test. Consequently, continuous plastic behavior around initial yield point was experimentally obtained by micro torsion test.

Fig. 3 shows fitting curve of experiment and simulation. Torsion simulation was conducted for one example of actual torsion test. For elastic simulation, initial gradient of load–displacement curve is almost the same. Initial yield point is defined separation point of load–displacement curve of experiment and elastic simulation. In this study, load–displacement curve of displacement until 600 nm was used for parameter fitting by least-square method because load is enough saturated at 600 nm. In this test, stage II

Table 1
Cu material parameter for the single crystal excluding fitting parameters.

Parameter	Value
Set of slip system	{1 1 1}<1 1 0>
Elastic modulus (GPa)	C_{11} = 168.4, C_{12} = 121.4, C_{44} = 75.4
The rate of sensitivity exponent	n = 50
Reference strain rate	$\dot{a}$ = 0.001 s^{-1}