Title	顕微ナノメカニックス計測法による金ナノ接点の弾性・塑性応答の解析
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Abstract

Study of elastic and plastic responses of gold nanocontacts using microscopic nanomechanical measurement method

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In this thesis, the elastic and plastic responses of gold nanocontacts (NC) was invested by microscopic nanomechanical measurement method (MNMM). Specifically, for the elastic response, we estimated the local Young's modulus of the internal local regions of the Au NCs. For the plastic response, we estimated the critical resolved shear stress (CRSS) required for slip to occur in the Au NCs. The Au NCs were fabricated using our developed in situ TEM holder, which is equipped with a quartz length-extension resonator (LER) as a force sensor for directly evaluating the force gradient (spring constant).

For nanocrystals, the Young's modulus exhibits both orientation dependence and size dependence. In devices made from nanomaterials, distribution of local Young's modulus is non-uniform. It is important to measure the local Young's modulus of nanocrystals. Our approach is based on the idea that under uniform shape and size conditions, a material with uniform Young's modulus will undergo uniform deformation under stress. However, if the Young's modulus is non-uniform, the deformation in different regions will vary. By measuring the local strain and its ratio to the overall strain, we can estimate the local Young's modulus for each region. Using our self-developed in situ TEM holder, we stretched Au NCs and observed their crystal structure through TEM, precisely measured the evolution of lattice spacing to obtain the local strain. Notably, the pixel size of the CCD we use is approximately 25 pm, while the maximum elastic elongation of the Au lattice is less than 10 pm, much smaller than the size of a single pixel. As a result, traditional methods cannot capture the elongation of the Au lattice. We fully utilized the large number of pixels in the TEM images and assumed that the TEM intensity follows a Gaussian distribution, enabling sub-pixel measurement of the Au lattice positions. In this way, we obtained the elongation of local regions during stretching. Additionally, we directly measured the force gradient (spring constant) applied to the Au NCs using FM method, and with the geometric information observed from TEM, we successfully estimated the local Young's modulus and studied its size dependence.

When the amount of stretching exceeds the material's elastic limit, it transitions from elastic deformation to plastic deformation. In nanocrystals, plastic deformation primarily occurs in the form of slip, and the necessary shear stress required for slip to occur in the slip direction is called as the CRSS. For bulk materials, the yield limit can be estimated by measuring the stress-strain curve. However, for nanomaterials, both stress and strain are extremely small, making direct measurement very difficult. We captured the energy dissipation associated with plastic deformation to estimate the maximum elastic deformation of Au NCs. Using the geometric information observed through TEM and the mechanical response obtained from FM method, we estimated the yield stress of Au nanocontacts with various size and orientation. For [110] Au NCs, with conductance values of 60

G_0 and 30 G_0, the yield stress was $2.0 \pm 0.1\ GPa$, regardless of size. In contrast, for [111] Au NCs with conductance of 30 G_0, the yield stress was $3.0 \pm 0.1\ GPa$. Considering the partial slip system in FCC metals, we found that the Schmid factor for [110] direction Au nanocontacts is $\sqrt{2}/3$ (≈ 0.47), the CRSS was calculated to be $0.94 \pm 0.1\ GPa$. Similarly, for [111] direction Au nanocontacts, the Schmid factor is $2\sqrt{2}/9$ (≈ 0.31), yielding an estimated CRSS of $0.94 \pm 0.1\ GPa$. These two results are consistent. Therefore, we conclude that the CRSS for the $\{11\bar{1}\}\langle 112\rangle$ slip system in Au NCs is $0.94 \pm 0.1\ GPa$.

In conclusion, a method for estimating the elastic and plastic responses of nanomaterials has been proposed. We studied Au NCs as an example, and our results had shown unique properties from bulk Au. This method is expected to be improved by introducing aberration-correct device to obtain better TEM resolution. The understanding of mechanics in atomic scale provide essential information for fundamental understanding and applications such as atomic scale nanodevices.

Keywords: nanomechanical, in-situ TEM, local Young's modulus, CRSS, dissipation energy.