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Size-Dependent Equilibrium Shape of Co-Cr Particles in Cu

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The equilibrium shape of particles embedded in a matrix is usually dominated by the elastic strain energy at large size while the interface energy becomes important at small size. Therefore, a systematic change in shape with increasing particle size is attributed to the increasing influence of elastic strain energy. Using conventional electron microscopy, we conduct experimental observations of coherent Co-Cr particles in a Cu matrix and demonstrate the evolution of the equilibrium shape of particles as a function of size ranging from 5nm to 50nm. Then the equilibrium shape change from sphere to cuboid is explained by considering anisotropic elasticity of the particles.

Typical distribution of Co-Cr particles are shown in FIG. 1a. It is found that the Co-Cr particles have intermediate shapes between sphere and cuboid. The observed intermediate shapes can be described as superspheres schematically illustrated in FIG. 1b where the x_i axes are parallel to the $\langle 100 \rangle$ direction of the particles. We then defined the shape parameter η as a ratio d/a in FIG. 1b and the characteristic radius r as a radius of an equivalent sphere of the same volume, respectively. A plot of the shape parameter η versus the characteristic radius r for more than 700 particles is shown in FIG. 2. It is apparent that the shape of particles changes from sphere to cuboid with increasing size.

Considering the sum of the elastic strain energy and the interface energy associated with the superspherical particles, the explanation of the equilibrium shape transition from sphere to cuboid is attempted. To accomplish this object, the simplified energy analysis proposed by Onaka et al. [1, 2] is adopted. Applying the energy minimizing condition, the parameter η representing the equilibrium shape can be formulated by

$$\eta \approx 1 + kC_{44}\frac{\varepsilon^2}{\gamma_{\mathrm{I}}}r \tag{1}$$

as a linear function of the characteristic radius r. Here, ε is the misfit strain, γ_{I} the isotropic interface energy, and the dimensionless parameter k is defined as the function of the elastic stiffness constants C_{11}, C_{12} and C_{44}. The least-square fit of the experimental data is shown as a solid line in FIG. 2. Using this result and substituting the appropriate values $k = 4.67\text{x}10^{-2}$, $C_{44} = 75.4$GPa, and $\varepsilon = 0.018$ (experimentally obtained), we can evaluate the Co-Cr/Cu interface energy as 290mJ/m^2. This value is about 1.5 times greater than the interface energy of Co/Cu, and is reasonably understood as the effect of Cr addition into the Co particles. It is concluded that the simplified energy analysis is well applicable to explain the experimental results on the systematic shape change of the Co-Cr particles in Cu.

References

[1] S. Onaka et al., *Mech. Mater.*, in press.
[2] S. Onaka et al., *Intermetallics*, in press.
[3] This research was partially supported by Japan Society for the Promotion of Science, Grant-in-Aid for Encouragement of Young Scientists (A), 13750648.

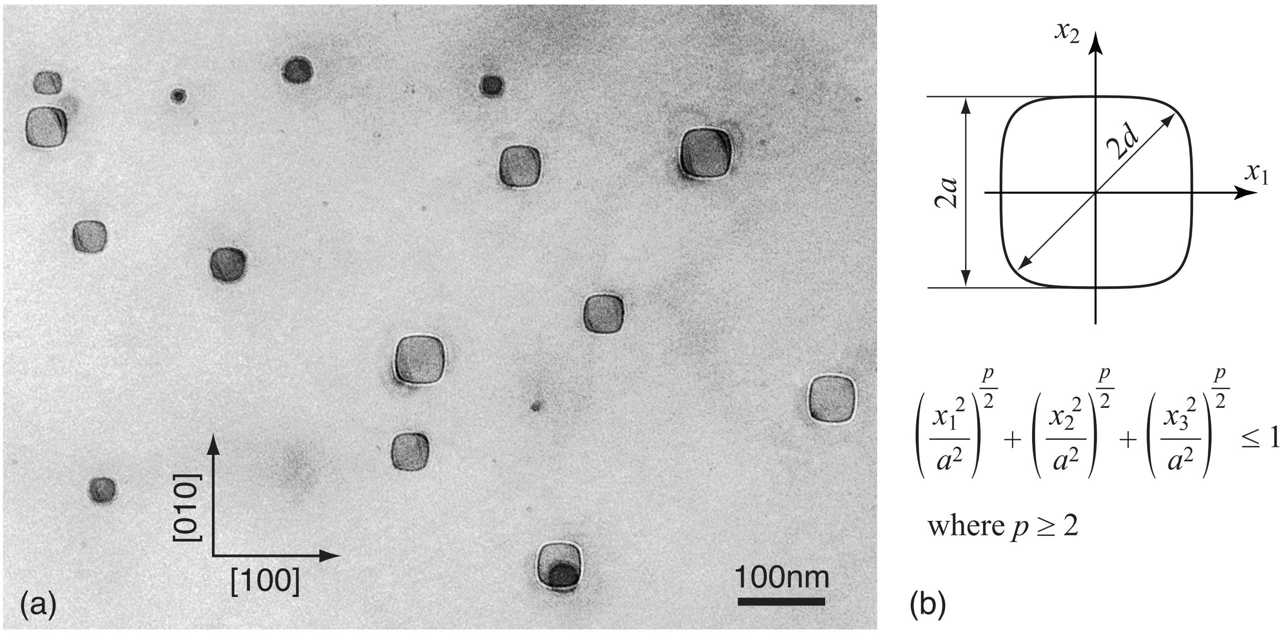

FIG. 1a. Transmission electron micrograph showing typical distribution of Co-Cr particles with superspherical shape in a specimen aged at 973K for 48h. To enhance perception of the shape of the particles, the off-axis condition where the strain-field contrast is almost invisible is adopted. FIG. 1b. Schematic illustration of the characteristic dimensions of the particles.

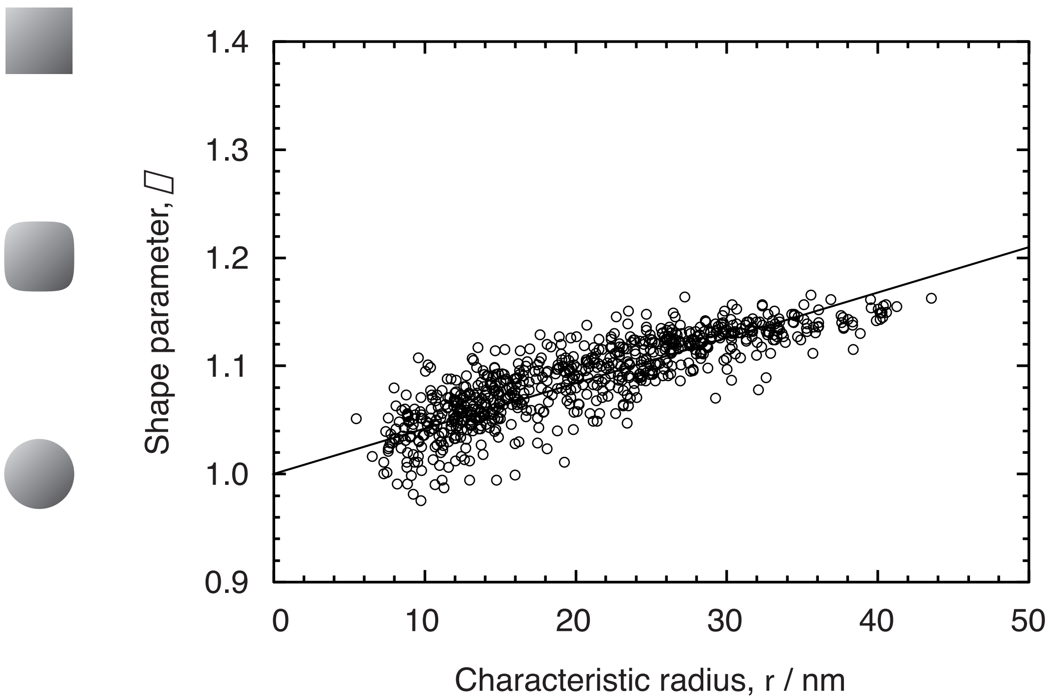

FIG. 2. Plot of the measured shape parameter □ as a function of characteristic radius *r*. The straight line shows the least-square fit of the data to Eq. 1. A series of particle shapes associated with □ are shown on the second axis.

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