Poster Presentation

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Ultra-high reciprocal resolution X-ray diffraction of Al and Cu

Tomoaki Sasaki[1], Hidetaka Kasai[2], Eiji Nishibori[2]
[1]*Graduate School Of Pure And Applied Sciences, University Of Tsukuba, Tsukuba, Japan,* [2]*Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan*
E-mail: s1630070@u.tsukuba.ac.jp

The bonding nature of Al and Cu have attracted large attention due to the relation between electron density and mechanical property [1,2]. Shear strength [1] and Young's coefficients [2] have been successfully explained for Al [1,2] and Cu [1] from theoretical charge densities. The shear strength of Al and Cu have been elucidated by the destruction and reconstruction of bonding [1]. Electron density distribution governs the mechanical properties of simple metals as described above.
Electron density is one of the most information rich observable and can be observed by X-ray diffraction measurement. We have developed experimental and analytical methods for accurate charge density study using multiple overlaid synchrotron radiation (SR) X-ray powder diffraction data at SPring-8. The accuracy of charge density determined by the method is comparable to that of very accurate Pendellösung method. Powder diffraction data measured at 3rd generation SR also applied accurate structural study of simple metals. Wahlberg et al. reported anharmonic thermal vibration of Cu from powder data measured at Petra-III [3].
We measured high resolution synchrotron powder X-ray diffraction data of Al and Cu at SPring-8 BL02B2 beamline. The wavelengths of the incident X-rays were 0.328 and 0.440 Å for Al and Cu, respectively. High energy X-ray were used for reduction of the effect of absorption and extinction. Bragg reflections in d>0.22 Å and 0.24 Å for Al at 30 K and Cu at 100 K were recognized in the powder profiles. We also measured in same 2θ range under 100, 200, 300, 400, 500, 600 K in Al and 300 K in Cu. Debye temperatures of Al and Cu are 398 and 315 K respectively. Therefore, these conditions cover the range from low temperature to Debye temperatures. Accurate structural studies including charge density study and anharmonic thermal vibration analysis of these dataset are now in progress.
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