

Exploring substrate-induced phase transition in metallic chromium foil using X-ray absorption spectroscopy

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According to the recently established pressure-temperature phase diagram [1], only the solid body-centred-cubic (bcc) phase of chromium exists at room temperature and pressures up to 90 GPa. However, it is known that chromium adopts a slightly distorted hexagonal close-packed (hcp) structure in Cr/Ru(0001) superlattices with the Cr layers thinner than 8 Å [2]. In this study, we have focused on the atomic structure and lattice dynamics of high-purity metallic chromium foils with two different thicknesses: the thick foil (5 µm) was substrate-free, while the thin foil (2 µm) was produced on a polyester substrate.

X-ray diffraction experiments were conducted for the thinner chromium sample using a Rigaku MiniFlex diffractometer before and after substrate removal by thermal heating. X-ray absorption spectroscopy experiments were performed for both samples over a temperature range of 10-300 K at the DESY PETRA-III P65 beamline (Hamburg, Germany) [3] in transmission mode at the Cr K edge. Advanced analysis of the extended X-ray absorption fine structure (EXAFS) spectra was carried out using the reverse Monte Carlo (RMC) method [4].

We found that the presence of an organic substrate induces a structural phase transition in the metallic chromium foil from a bcc to a hcp phase, presumably due to mechanically induced strain. The atomic coordinates obtained from RMC simulations of EXAFS spectra were used to obtain the mean-square relative displacements (MSRDs) for the Cr-Cr atomic pairs. The MSRD values for the thick chromium foil in the bcc phase are consistent with the literature data [5]. Furthermore, the analysis of the MSRDs suggests that, unlike bcc chromium, the lattice dynamics of hcp chromium is strongly anisotropic. Finally, the MSRD values of hcp chromium were compared to those of several other hcp (Co, Ti, Zr, Zn, Cd) and bcc (Mo) metals.

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References

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