# Anomalous Debye-Waller Factor in Epitaxial fcc Co(001) Film

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## Introduction

The element cobalt undergoes a structural transformation from the hexagonal closed-packed (hcp) form to the face-centered cubic (fcc) modification at about 700K. The transformation is displacive (i.e., it involves the collective movement of a large number of atoms). Structural transitions are often governed by the softening of a particular lattice vibration, the so-called "soft mode," which triggers the transition. However, in single-crystal Co [1] and in slightly Fe-enriched Co [2], no sign of a soft mode could be detected by inelastic neutron scattering. Only the decrease of the shear constant $c_{44}$ [3] can be taken as a precursor effect to the transformation. Therefore, models involving local strain embryos [4] or a peculiar dislocation arrangement [5], which do not show up in the phonon dispersion, are favored as an explanation.

The transition is especially sensitive to metallic impurities and external pressure [6] (e.g., the transformation temperature can be increased by 200K upon a *hydrostatic* pressure of 50 kbar). An external *biaxial* strain can be imposed by a coherent substrate in epitaxial growth. Since a film that adheres well is clamped by the substrate in two directions, it can be expected that a transformation involving a shear that is not parallel to the substrate-film interface may be hindered or even suppressed. In particular, the transformation mechanism in the presence of an external strain or a substrate potential will be different from that in the bulk.

## Methods and Materials

The samples under investigation have been prepared by MBE by using electron beam evaporators. A 100-Å-thick Cu(001) buffer layer was deposited onto a SrTiO3(001) substrate at room temperature (RT). The buffer was annealed at 650K, then the 500-Å fcc Co film was deposited again at RT. The sample was transferred in air and cleaned in ultrahigh vacuum (UHV) by moderate sputtering and then successively annealed to up to 650°C°, 200°C above the bulk transition temperature. Line scans parallel to the fcc(111) direction should reveal the hcp stacking faults accompanying the structural transition (see Fig. 1).

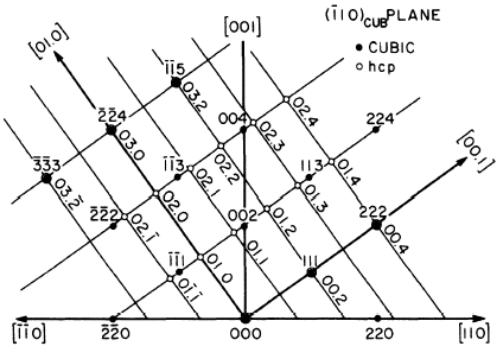


*FIG. 1. Reciprocal lattice of the fcc and hcp structure. Solid dots represent fcc reflections, and open circles represent hcp reflections.*

## Results

Figure 2 shows typical scans parallel to the [111] direction for different temperatures. Only the fcc Co reflections are visible, together with a small contribution from a nearby substrate truncation rod. No signs of hcp stacking faults at the expected 1/3 and 2/3 positions are visible. Since the sample remained in the metastable fcc phase in the entire temperature region (RT of 920K), we resorted to the measurement of the thermal Debye-Waller factor upon cooling the sample. The intensities of the fcc (222), (333), and (444) reflections were determined by integrating angular and radial scans. The results for 11 temperatures on the cooling curve are shown in Fig. 3, together with the lattice parameter of the Co film. An anomaly at 300°C is clearly visible, accompanied by a change in slope.

## Discussion

We think of two different possible origins of the metastability of the fcc phase. The film could be stabilized by impurities or defects, or the fcc-hcp transition could be blocked by the clamping of the substrate. In either case, the anomaly in the thermal movement of the Co atoms is remarkable. We are currently trying to separate the thermal Debye-Waller factor from a static one due to defects by extending the measurements below RT down to 20K. In parallel, we are determining the impurity concentration by Rutherford backscattering spectroscopy.

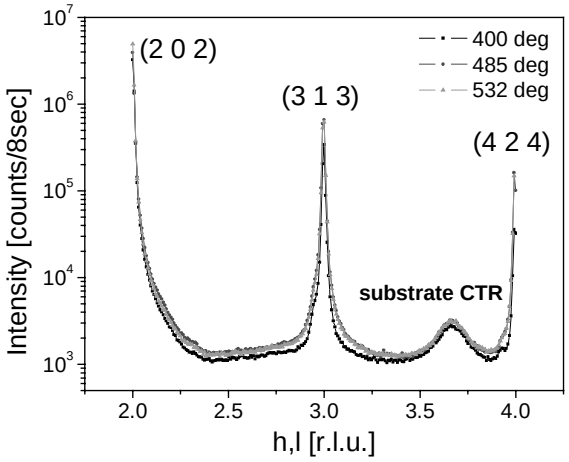


*FIG. 2. Scan parallel to the [111] direction of the fcc cobalt lattice for three temperatures.*

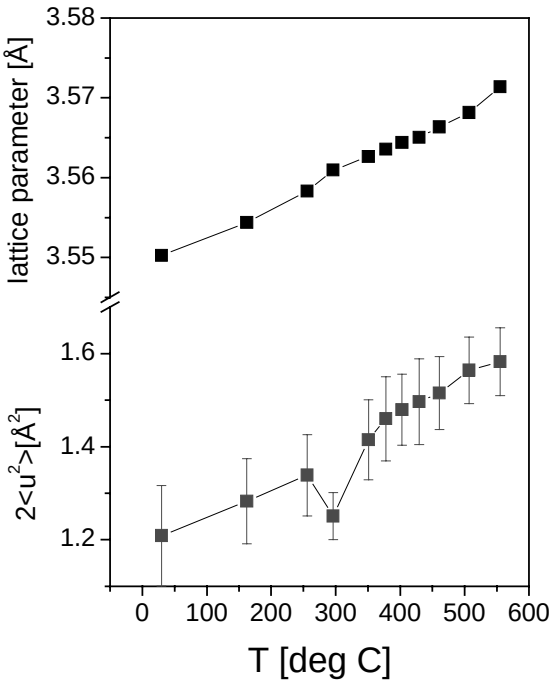


*FIG. 3. Mean square displacement and lattice parameter as a function of temperature.*

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