Nanoscale Diagnostics of Crystal Surface Layers Displacement with X-ray Standing Wave Technique

E. Sozontov, [1] V. Kohn, [2] A. Kazimirov, [3] J. Zegenhagen[4]

[1]Institute of Crystallography (Kaluga Branch) RAS, Kaluga, Russia; [2]Russian Research Center "Kurchatov Institute", Moscow, Russia; [3]CHESS, Ithaca, NY, U.S.A.; [4]ESRF, Grenoble, France

Introduction

Advanced nanoscale technology needs adequate diagnostic tools. The X-ray standing wave (XSW) technique is meanwhile recognized as a powerful tool for surface and interface crystal structure analysis with high accuracy.

Methods and Materials

In a different approach [1, 2] we are using the interference field (standing wave), generated inside a single crystal substrate via Bragg diffraction, as a basis to measure the negligible shift of the surface atomic planes of an epitaxial overlayer that is caused by the cumulative effect of the lattice constant difference of the N underlying lattice planes of the overlayer. In this way, the interference field, generated by the single crystal substrate and therefore periodic with the substrate lattice, serves as a precise Ångstrom-scale benchmark for the lattice positions of the surface layers of an epitaxial overlayer.

We used this approach and theoretical evaluations [3] to measure the isotopic mass dependence of the lattice constants of Si and Ge. An isotopically enriched ^{30}Si film was grown on a single crystal substrate with natural isotopic composition by liquid phase epitaxy. The isotopically enriched ^{76}Ge film was grown by molecular beam epitaxy on a highly isotopically enriched ^{70}Ge single crystal substrate. The XSW, generated by the substrate, serves as a reference for the lattice planes of an epilayer of different isotopic composition.

Results and Discussion

The x-ray standing wave (XSW) technique was used to measure the isotopic mass dependence of the lattice constants of Ge. Using molecular beam epitaxy (MBE), the 1 μm thick ^{76}Ge film was grown on the (111) surface of an isotopically pure (99%) ^{70}Ge crystal. However, this single crystal was grown by the Bridgeman technique with a corresponding moderate crystalline quality prohibiting standard XSW measurements. With the crystal mounted on a flow-through cryostat and detecting electrons from the overlayer by a channeltron we performed XSW mesurements at the RÖMO (HASYLAB) station in backscattering geometry at a Bragg angle of 89.9° in the temperature range from 30K to 300K. The surface planes of the ^{76}Ge layer move inward by about d(444)/2 = 40 *pm* upon lowering the temperature from 300 to 30K. From this value, a change of the lattice constant difference between ^{76}Ge and ^{70}Ge can be calculated. Scaled to ΔM =1 *amu* we find (Δa/a) of -3.6×10^{-6} and -8.8×10^{-6} for Ge at 300 and 30K, respectively.

We employed the same technique to measure the lattice constant difference of silicon isotopes with high accuracy. For this experiment an isotopically enriched Si film (60% ^{30}Si, 40%^{28}Si) was grown on natural Si(111) by liquid phase epitaxy. The thickness of the film and the isotopic composition were determined accurately by RBS and SIMS, respectively. The XSW measurement was performed at HASYLAB/DESY, emploing a (333) reflection from the Si with an X-ray energy of 9.5 keV. The results of the measurement are shown in Fig.1 in comparison with two theoretical calculations [4, 5]. We believe that the accuracy of our results represents a stringent test for theory and may stimulate calculations exhibiting a higher accuracy.

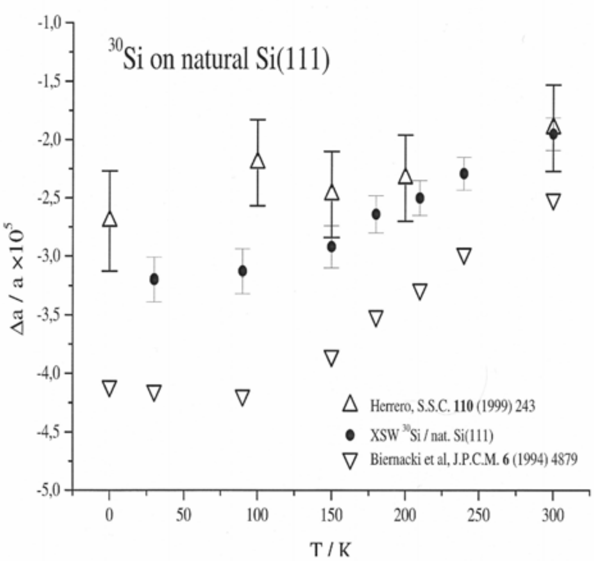

Fig. 1.

In conclusion, emploing XSW and photoemission, the displacement of the surface planes is determined from which the lattice constant difference Δa is calculated. Scaled to ΔM =1 *amu* we find (Δa/a) of -3.6×10^{-6} and -8.8×10^{-6} for Ge and -1.8×10^{-5} and -3.0×10^{-5} for Si at 300 and 30 K, respectively, in good agreement with published calculations.

[1] A. Kazimirov, J. Zegenhagen, M. Cardona, Science 282, 930, (1998).
[2] E. Sozontov, L.X. Cao, A. Kazimirov, V. Kohn, M. Konuma, M. Cardona, J. Zegenhagen, Phys. Rev. Lett. 86, 5329 (2001).
[3] V. Kohn, Phys. Stat. Sol. (b), 231, 132 (2002).
[4] S. Biernacki, M. Scheffler, Journ. of Phys. Cond. Matter 6, 4879 (1994).
[5] C. Herrero, Solid State Comm. 110, 243 (1999).