SURFACE THERMAL EXPANSION[1]

Ismail,[2] Ph. Hofmann,[3] A. P. Baddorf, D. M. Zehner, and E. W. Plummer[4]

The creation of a surface breaks the translational symmetry of the bulk with the electrons redistributing to lower their energy, resulting in a new lattice structure. Surface relaxation and reconstruction have been studied for years, and it is generally assumed that theory and experiment are in fairly good agreement for the ground state properties at a metal surface. There is a conceptual picture of the origin of the interplanar relaxation and the dependence of this relaxation upon the openness of the surface. However, when it comes to finite temperature behavior such as thermal expansion, there is no reliable model, and glaring discrepancies exist between theory and experiment.

The temperature-dependent interlayer spacing for Mg(0001), Mg(10$\bar{1}$0), and Be(10$\bar{1}$0), have been measured. The new data have been compared with all existing surface thermal expansion data in an attempt to identify simple principles governing the thermal behavior. Mg(0001), as with the case of other close-packed metal surfaces, exhibits a slight enhancement in the thermal expansion of d_{12} compared with the bulk. In contrast, the open surfaces, Mg(10$\bar{1}$0), and Be(10$\bar{1}$0), exhibit oscillatory thermal behavior for Be(10$\bar{1}$0). A normalized interlayer thermal expansion coefficient α_{ij} can be defined as $\alpha_{ij} = \{d_{ij}(T) - d_{ij}(0)\}/d_{ij}(0)T$. Figure 1 shows the behavior of α_{12} for all of the data in the literature as a function of the normalized area A_0 of the surface unit cell. For the close-packed surfaces ($1/A_0$ is ~0.9), all surfaces show a small thermal expansion, but for open surfaces ($1/A_0 < 0.6$), there is a dramatic difference between different materials. A clue to this behavior was discussed theoretically. Thermal contraction in d_{12} is always accompanied by thermal expansion in d_{23}. In fact, when α_{13+} is plotted, all materials have approximately an order of magnitude smaller thermal expansion coefficient.

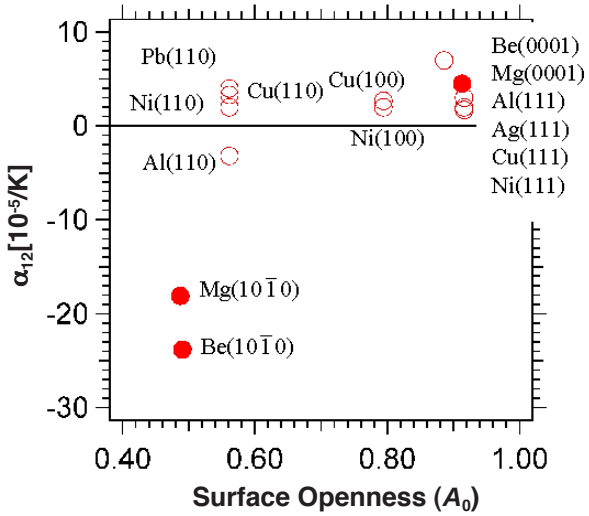

Fig. 1. Measured surface thermal expansion in the first interlayer spacing as a function of the openness of surface ($1/A_0$), where $A_0 = A_s/V_0^{2/3}$. A_x is the area of the surface unit cell. The solid points were measurements by the group.

It was shown theoretically that the charge redistribution at the surface accompanied by the lattice relaxation [for fcc(110) surfaces] dramatically increases the NN force constants between the first and third layer and reduces the NN force constant in the plane making d_{13} rigid. It is clear that in the environment of the surface (broken symmetry), thermal expansion (contraction) can occur without anharmonicity in the interplanar potential.

---

1. Summary of papers: *Phys. Rev. B* **62**, 17012 (2000); *Phys. Rev. B* **63**, 233401 (2001); *Surface Science Letters* (in press).
2. Postdoctoral research associate from The University of Tennessee (funded by NSF DMR 0105232).
3. University of Aarhus, Aarhus, Denmark.
4. ORNL/UT Distinguished Scientist.
5. S. Narasimhan, *Phys. Rev. B* **64**, 125409 (2001).