Rumpled Relaxations of TiC(001) and TaC(001) Determined by High-Resolution Medium Energy Ion Scattering Spectroscopy

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Abstract

The rumpled relaxations of TiC(001) and TaC(001) with strong covalent bonds were determined precisely by medium energy ion scattering using a new toroidal electrostatic analyzer with an excellent energy resolution of $\Delta E / E = 9 \times 10^{-4}$. It allows a monolayer depth resolution and thus a simple triangulation method using the ion shadowing effect achieved the accuracy of 0.01 Å in depth for the displacement of atoms near a surface region. The surface relaxation (+ : outwards) and rumpling (+ : displacement of C toward vacuum side larger than that of Ti(Ta)) were estimated to be $+0.1 \pm 0.3$ % and $+3.5 \pm 0.5$ % for TiC(001) and $+1.4 \pm 0.3$ % and $+4.9 \pm 0.5$ % for TaC(001). The present result is consistent with the recently reported calculation using the full-potential linear muffin tin orbital method but inconsistent with the predictions using the tight-binding model and the full-potential linearized augmented plane wave method.

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