Surface Structure and Lattice Dynamics of Alkali Halide Crystals Studied by High-resolution Ion Scattering and Molecular Dynamics Simulation

Tetsuaki Okazawa

The rumpled surface structure and thermal lattice vibrations of KI(001) and RbI(001) were analyzed directly by high-resolution medium energy ion scattering (MEIS). The relaxation of interlayer distance between the top- and 2nd-layer and the rumpling of the top- and 2nd-layers were determined using the ion shadowing effect with an accuracy of 0.01Å. From the displaced lattice positions determined above, we derived the dipole moments of the top- and 2nd-layer ions self-consistently employing the polalizabilities estimated from the optical refractive index combined with the Clausius-Mossotti relation. The present MEIS results are relatively in good agreement with the shell model calculations and the molecular dynamics (MD) simulations for both RbI(001) and KI(001) and also consistent with the *ab initio* calculation for RbI(001). We also determined the root-mean-square (rms) thermal vibration amplitudes (TVA) of the bulk and the top-layer ions together with the correlations of the ions in the [001]- and [101]-strings by taking various kinds of scattering geometries. The bulk TVAs determined by MEIS are almost mass-independent, in contrast to those calculated from the Debye approximation, which leads to TVAs proportional to $M^{-1/2}$. As expected, we observed strong correlations in the direction perpendicular to the [001]-string but small ones in the motion perpendicular to the [101]-string. The results obtained were compared with those calculated from MD simulations based on a classical model using the above dipole moments and the Born-Mayer-type pair potential. The present results are in overall agreement with the MD simulations employing the pair potential proposed by Catlow *et al*.