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

Yoshiaki Kido*, Yoshihiro Yagi and Tetsuaki Okazawa

Abstract

The rumpled surface structure and thermal lattice vibrations of KI(001) and RbI(001) were measured 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 balance between a short-range force and a long-range Coulombic one made it possible to judge the applicability of the short-range pair potentials proposed so far. We also determined the root-mean-square (rms) thermal vibration amplitudes 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 results obtained were compared with those calculated from the molecular dynamics (MD) simulations based on a classical model using the dipole moments determined above and the Born-Mayer-type pair potential. The present MEIS results are in over-all agreement with the MD simulations.

Department of Physics, Ritsumeikan University, Kusatsu, Shiga-ken 525-8577, Japan

* Tel/Fax: +81-77-561-2710/2657, E-m: ykido@se.ritsumei.ac.jp