

11-3-1986

Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions

L. L. Boyer

University of Nebraska - Lincoln

M. J. Mehl

University of Nebraska - Lincoln

J. L. Feldman

University of Nebraska - Lincoln

John R. Hardy

University of Nebraska - Lincoln

J. W. Flocken

University of Nebraska - Lincoln

See next page for additional authors

Follow this and additional works at: <http://digitalcommons.unl.edu/physicshardy>



Part of the [Physics Commons](#)

Boyer, L. L.; Mehl, M. J.; Feldman, J. L.; Hardy, John R.; Flocken, J. W.; and Fong, C. Y., "Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions" (1986). *John R. Hardy Papers*. 36.

<http://digitalcommons.unl.edu/physicshardy/36>

This Article is brought to you for free and open access by the Research Papers in Physics and Astronomy at DigitalCommons@University of Nebraska - Lincoln. It has been accepted for inclusion in John R. Hardy Papers by an authorized administrator of DigitalCommons@University of Nebraska - Lincoln.

Authors

L. L. Boyer, M. J. Mehl, J. L. Feldman, John R. Hardy, J. W. Flocken, and C. Y. Fong

ERRATA

Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions. L. L. BOYER, M. J. MEHL, J. L. FELDMAN, J. R. HARDY, J. W. FLOCKEN, and C. Y. FONG [Phys. Rev. Lett. **54**, 1940 (1985)].

In our recent Letter we introduced an *ab initio* model for spherically symmetric charge relaxation of ions in a crystal, called potential-induced breathing (PIB), and demonstrated its importance in the calculation of elastic constants. We also investigated the splitting of the longitudinal optic (LO) and transverse optic (TO) mode frequencies, which results from the macroscopic field associated with longitudinal modes. In the discussion immediately before and after Eq. (5) we argued, incorrectly, that the only contributions to the LO-TO splitting from PIB were from terms involving S'_k , the derivative of the self-energy of the k th ion with respect to the electrostatic potential at the k th-ion site. In fact, other terms within the PIB model contribute as well. Further study has shown that the treatment of macroscopic field effects in the PIB model is not straightforward. This will be discussed in a future paper (R. E. Cohen, L. L. Boyer, and M. J. Mehl, to be published).