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Role of spatial dispersion in formation of pure-shear elastic surface waves in crystals

V. V. Krylov

M. V. Lomonosov State University, Moscow

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Several authors (e.g., Refs. 1–5) have recently discussed the existence of "nonclassical" pure-shear elastic surface waves in crystals. On the basis of the dynamic theory of the crystal lattice, Aldredge\(^1\) and Gel'f'gat\(^2\) have shown that the influence of discreteness of the lattice leads to the existence of slightly inhomogeneous transverse surface waves in a number of chosen directions in cubic crystals, and that their amplitudes decay with depth as \(\sim d^2\), where \(d\) is the lattice constant and \(k\) is the wave number. Lyubimov\(^3\) and Vusheva\(^4\) gave a phenomenological analysis of the existence of pure shear surface waves in the approximation of weak spatial dispersion. In contrast with Refs. 1 and 2, their calculations indicated that pure shear surface waves cannot be propagated in centrosymmetric crystals. However, by going to the long-wave limit in the lattice dynamic equations, Gel'f'gat\(^5\) has recently shown that the standard form of the boundary conditions \(\tau_{ij}\mid_1 = 0\), used in a number of phenomenological investigations including Refs. 3 and 4, is valid only in the local theory of elasticity, and that a certain modification of this in the case of weak spatial dispersion, directly following from the microscopic theory, is responsible for the existence of pure shear surface waves. From a somewhat different viewpoint, the possibility of existence of slightly inhomogeneous pure shear surface waves in crystals was demonstrated by Krasi'n'nikov and Krylov,\(^6\) who supplemented the usual boundary conditions by terms phenomenologically representing the influence of surface tension in crystals (see also Ref. 7) and the changes in the force constants and density in the surface layers of atoms. The surface waves in this case are in no way associated with spatial dispersion.

I shall show that the results in Refs. 1, 2, and 5 are essentially equivalent to those in Ref. 6, since the boundary conditions obtained in Ref. 5 are a particular case of the conditions in Ref. 6. In this connection we may note that in my opinion, the assertion in Ref. 5 that the existence of the surface waves is associated with weak spatial dispersion is not altogether correct, since, as we shall see, the latter is effective only in higher approximations in respect of \(d\).

To verify this we shall use the so-called semiphenomenological approach, by distinguishing a surface layer of atoms in the crystal, with a thickness approximately equal to \(\sim d\). If no account is taken of surface distortions, the linearized equation of state of the crystal, which is valid both in the surface layer and in the bulk, can be repre-

sentated with the aid of an operational relation of the strongly nonlocal theory of elasticity\(^6\):}

\[
\tau_{ij}(x,y,z) = \sum_{l} \sum_{j} \epsilon_{ijkl}(x',y',z',x)u_{kl}(x',y',z') \delta x' \delta y' \delta z',
\]

where \(\tau_{ij}\) are the components of the elastic stress tensor, \(u_{ij}\) is the displacement vector, and \(\epsilon_{ijkl}\) is the nucleus of the nonlocal elastic moduli. In (1) it is important to note that owing to the presence of the boundary, the integration with respect to the normal coordinate \(z\) is carried out only over half the real axis. The approximation of weak spatial dispersion is easily obtained from Eq. (1) with the aid of expansion of \(u_{ij}\) in a power series in the neighborhood of the point \((x, y, z)\), taking account of the first two nonvanishing terms. In the zero or local approximation, we obtain the following equation of state:

\[
\tau_{ij}(x,y,z) = \sum_{l} \sum_{j} \epsilon_{ijkl}(x',y',z') \delta x' \delta y' \delta z',
\]

from which it follows that for points in the surface layer the corresponding local moduli \(c_{ijkl}(x)\), which are triple integrals on the right-hand side of (2), are less than the same moduli in the bulk of the crystal (in the latter case, in view of the narrowness of the nucleus \(\epsilon_{ijkl}(x',y',z')\) which has characteristic width of about \(\sim d\), the influence of the boundary is not important). This fact has a very simple interpretation. In fact, roughly speaking, the elastic forces acting on each surface atom are due to a smaller number of atoms than in the case of the interior of the crystal. As a result, there is a decrease in the local elasticity moduli in the surface layer. It was this effect, in no way connected with weak spatial dispersion, which was taken into account in Ref. 6 with the aid of phenomenologically derived surface elasticity moduli understood in the sense of Gibbs. The corresponding macroscopic boundary conditions for a centrosymmetric crystal, taking account of changes in the elasticity moduli in the surface layer of atoms, are easily obtained directly from Eq. (2) with the aid of a variation procedure described in Refs. 6 and 7:

\[
\gamma(x,y) = c_{ijkl}(x) - c_{ijkl}(x) = 0.
\]

Here \(c_{ijkl}^s = \int_{-d}^{0} [c_{ijkl}(s) - c_{ijkl}(0)] ds\) are the surface elasticity moduli, understood in the sense of Gibbs, and \(c_{ijkl}\) are the values of the local elasticity moduli in the bulk of the crystal.
Crystal structure of synthetic fluoropyromorphite Pb$_5$[PO$_4$]$_3$F

E. L. Belokoneva, E. A. Troneva, L. N. Dem'yanets, N. G. Duderov, and N. V. Belov

Institute of Crystallography, Academy of Sciences of the USSR
and M. V. Lomonosov State University, Moscow

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The authors have made an x-ray structural investigation of synthetic lead phosphate obtained in hydrothermal conditions in the system PbO – Pb$_3$O$_4$ – KF – H$_2$O. The Pb/P ratio was varied by introducing various amounts of potassium phosphate. The principal crystalline phase formed over wide ranges of the ratio Pb$_3$O$_4$/PbO (1 : 4 to 3 : 1 in moles) of the KF concentration (5–30 mass %) was lead phosphate which was attributed, according to its interplanar distances (Table 1), to a structural analog of pyromorphite Pb$_3$[PO$_4$]$_3$X (ASTM), where usually X = OH or Cl. The results of differential thermal and gravimetric analyses supported the conclusion that there were no hydroxyl groups in the synthesized compound; and on the basis of the valence balance the formula of the synthesized phosphate can be written in the form Pb$_5$[PO$_4$]$_3$F. It is stable when heated to 1200°C, and there are no thermal effects on the DTA curve up to the melting point.

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Translated by S. G. Kirsch