The role of spatial dispersion in the formation of purely shear surface elastic waves in crystals

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BRIEF COMMUNICATIONS

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

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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, Aldridge and Gel'fand 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 and Vyazmina 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'fand has recently shown that the standard form of the boundary conditions \( \Gamma_{ij} = 0 \), 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 Krasil'nikov and Krylov, 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-
crystal. Since it follows from (2) that the moduli $c_{ijkl}(z)$ differ from their bulk values only in a thin surface layer with a thickness of about $\sim d$, it is obvious that $c_{ijkl} \sim d\{c\}$, where $c$ is the maximum value of $c_{ijkl}$. The reader will remember that in the surface layer $\left|c_{ijkl}(z) - c_{ijkl}\right| \sim \left|c_i\right|$. Expression (3), which is a particular case of the boundary conditions in Ref. 6 in which no account is taken of the influence of surface tension and changes in the distances between the planes of atoms in the surface layer, takes the same form as the conditions derived in Ref. 5 from the lattice model. The tensor $\hat{c}_{ijkl}$, preceding the quantities $u_{k_{ij}}$ in Ref. 5, obviously has the meaning of the above surface elastic moduli $c_{ijkl}$. Owing to the presence of a relation between the individual components of the deformation tensor, due to the free boundary (for details see Ref. 9), in describing the deformation state of the surface layer it is sometimes convenient to assume that the indices $k, l$, and $u_{k_{ij}}$ take only the surface values $x$ and $y$ (Ref. 6) (assuming that $|a| = 2a_p$). From the condition of static equilibrium of the crystal it follows that the renormalized values of $\hat{c}_{ijkl}$ are correspondingly nonzero only for surface values of $i$ and $j$.

Now let us consider the role of the approximations in the expansion of (2), representing the influence of spatial dispersion. Since the second term in the expansion of (2) is proportional to $d$ near the surface, it is obvious that in the case of centrosymmetric crystals this allowance leads only to a component of order $\sim d^2$ in the boundary conditions (3). Of course, for crystals without a center of symmetry, in boundary conditions (3) there appears an additional term of order $\sim d$, due to the second term in the expansion of (2) in the bulk of the medium. In this connection we must note that the conclusions drawn in Refs. 3 and 4 for noncentrosymmetric crystals are still qualitatively correct. But in crystals with a center of symmetry, including the cases discussed in Refs. 1, 2, and 5, the influence of the component of order $\sim d$ in the boundary conditions becomes crucial on account of changes in the elastic properties of the surface layer of atoms. The solution of the corresponding boundary-value problem for the equations of the theory of elasticity leads to the occurrence of pure shear surface waves with a decay law proportional to $\sim d^2$ (Ref. 6), which are in principle the same as waves of the Ilaive type in layered systems,6 or to linear dispersion of Rayleigh surface waves,7 occurring in the classical limit also ($d \rightarrow 0$). In this case, the influence of spatial dispersion is felt only at very high frequencies (of order $\sim 100$ GHz or more) at which it causes changes in the phase velocities of surface waves.


Translated by S. G. Kirsch

Crystal structure of synthetic fluoropyromorphite Pb$_5$[PO$_4$]$_3$F

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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—P$_2$O$_5$—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 P$_2$O$_5$/PbO (1: 4 to 3: 1 in moles) and 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$_4$]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$_3$[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.

| TABLE 1. Interplanar Distances in Pb$_5$[PO$_4$]$_3$F, Å |
|-----------------|-----------------|-----------------|
| d               | d + h           | d - h           |
| 4.31            | 14              | 2.32            | 1              | 1.719 | 1 |
| 4.10            | 17              | 2.19            | 9              | 1.883 | 1 |
| 3.71            | 17              | 2.43            | 5              | 1.626 | 1 |
| 3.23            | 17              | 2.040           | 20             | 1.600 | 5 |
| 2.92            | 20              | 1.988           | 10             | 1.583 | 10 |
| 2.62            | 20              | 1.866           | 25             | 1.542 | 8 |
| 2.42            | 20              | 1.866           | 12             | 1.492 | 10 |
| 2.35            | 25              | 1.938           | 25             | 1.383 | 25 |

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