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PHONON FOCUSING AND THE SHAPE OF THE RAY SURFACE IN CUBIC CRYSTALS

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Abstract.
A systematic study has been carried out on the dependence of the phonon ray surface of cubic crystals on elastic constants. The correspondence between folds in this surface and the presence of caustics in the flux of phonons emanating from a localised heat source is explored. The line, cusp, butterfly and hyperbolic umbilic elementary catastrophes as well as some remarkable types of structural instability are shown to occur in these caustics. A method is demonstrated for portraying the ray surface which provides an immediate indication of the number of separate components a ballistic heat pulse will split up into on propagating in various directions, and what the relative intensities and the spacings of these components will be.

1. Introduction.— In the long wavelength limit continuum elasticity theory can be used for calculating acoustic phonon phase and group velocities /1,2/. The information thus gained is conveniently displayed in the form of velocity (v), slowness (S) and ray (V) surfaces /3/. The ray surface is of central importance in phonon imaging /4-6/, in that it maps out the profile of a ballistic heat pulse one unit of time after it has emanated from a point source at the origin. This surface is commonly studied in conjunction with S. The two are polar reciprocals of each other and the ray vector for a phonon is normal to S. Moreover, phonon flux is inversely proportioned to the curvature of S /7/. Contours of zero Gaussian curvature (parabolic lines) in S give rise to folds in V and divergent phonon flux. At conical points the curvature of S is infinite. Such points map onto circles in V at which the two transverse sheets join up smoothly and the phonon intensity is zero. The folds in V form complex patterns which are a function of the crystalline anisotropy.

2. Cubic crystals.— The folding pattern here is determined by the elastic constant ratios \( a = C_{11}/C_{44} \) and \( b = C_{12}/C_{44} \). For stability a crystal has to lie in the wedge shaped area between the lines \( a = -2b \) and \( a = b \) in the \((a,b)\) plane. This area may be subdivided into a limited number of regions in each of which \( V \) possesses certain distinct topological features. For instance, between the lines \( b = 1 \) and \( 6(a-b+1)^2(b+1)-3(a-b-2)^2(b+1)-(a-b+1)(a-b-2)(8a+13b+5) = 0 \), the folding pattern shown in fig. 1b holds for the slow transverse \((T_2)\) sheet of \( V \). Fig. 1a shows the location of parabolic lines on \( S \) that map onto these folds. These lines separate regions of \( S \) which are convex (both principal curvature positive), saddle shaped (one curvature negative) and concave (both curvatures negative).
Fig. 1: Correspondence between (a) parabolic lines in $S$ and (b) folds in $V$ for slow transverse ($T_I$) phonons. The diagrams are limited to the vicinity of the irreducible sector of the unit sphere lying within the [001], [101] and [111] directions.

It is noteworthy that the parabolic lines which meet at the conical point are responsible for part of a fold edge which weaves back and forth between the $T_I$ and fast transverse $T_p$ sheets of $V$, meeting the conical circle tangentially where it makes the crossing. The integrated intensity across the caustic diminishes as the caustic approaches the conical circle, as can be seen in fig. 2.

The symbol $\hat{\nabla}$ is used to indicate the direction of the vanishing principal curvature. Where this is parallel to the parabolic line a cusp appears in the folding line of $V$, except at conical points where the aforementioned effect takes place. For certain values of the elastic constants 8 fold lines in the $T_I$ sheet of $V$ converge to a point in the $<100>$ directions. This represents a structurally unstable situation which results from the degeneracy of the $T_1$ and $T_2$ modes in these directions. On varying the elastic constants some of the higher elementary catastrophes are exhibited. A configuration of 3 cusps which coalesce into a single one in conformity with the butterfly catastrophe can be observed in the cube planes near the $<100>$ directions. The cusp then makes contact with a neighbouring fold line to give rise to the hyperbolic umbilic catastrophe.

Fig. 3 shows the pattern of fold lines in $V$ that obtains for the $T_I$ sheet when the anisotropy lies between the two lines $a^2+(a-1)(b+1)-2(b+1)^2-1 = 0$, and $(a-1)(a+b)+(a-b-2)(b+1)^2 = 0$. 

Fig. 2: Phonon enhancement map for $T_I$ phonons in CsCl. The points represent group velocity directions for a uniform distribution of wave normals on average $0.5^\circ$ apart.
Fig. 3: A folding pattern for the T<sub>1</sub> sheet of V.

Fig. 4: A polar section of the full ray surface of Ge for $\phi = 45^\circ$. The mode points denote ray vectors which lie within 0.5° of this plane.

Fig. 4 shows a $\phi = 45^\circ$ polar section of the full ray surface of Ge, a crystal which satisfies the above criterion. Sectioned fold edges appear as cusps in this diagram, and arrows indicate the position of the conical circle. Diagrams of this type, by the location and density of mode points, give an immediate indication of how a ballistic heat pulse can be expected to split up into components for propagation in various directions.

References