

ELASTIC WAVES IN CUBIC CRYSTALS

By considering as in Figs. 18 and 19 the forces acting on an element of volume in the crystal we obtain the equation of motion in the x direction

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z} ; \quad (55)$$

here ρ is the density and u is the displacement in the x direction. There are similar equations for the y and z directions. From (38) and (50) it follows that for a cubic crystal The X_x , X_y , and X_z will be substituted from eq. (38)

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial e_{xx}}{\partial x} + C_{12} \left(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x} \right) + C_{44} \left(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z} \right) ; \quad (56)$$

here the x, y, z directions are parallel to the cube edges. Using the definitions for e_{yy} , e_{xy} , e_{xz} (31) and (32) of the strain components we have

X

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2} + C_{44} \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 w}{\partial x \partial z} \right) , \quad (57a)$$

where u, v, w are the components of the displacement \mathbf{R} as defined by (29).

The corresponding equations of motion for $\partial^2 v / \partial t^2$ and $\partial^2 w / \partial t^2$ are found directly from (57a) by symmetry:

Y

$$\rho \frac{\partial^2 v}{\partial t^2} = C_{11} \frac{\partial^2 v}{\partial y^2} + C_{44} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 w}{\partial y \partial z} \right) ; \quad (57b)$$

Z

$$\rho \frac{\partial^2 w}{\partial t^2} = C_{11} \frac{\partial^2 w}{\partial z^2} + C_{44} \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z} \right) . \quad (57c)$$

We now look for simple special solutions of these equations.

Waves in the [100] Direction

One solution of (57a) is given by a longitudinal wave


$$u = u_0 \exp [i(Kx - \omega t)] , \quad (58)$$

where u is the x component of the particle displacement. Both the wavevector and the particle motion are along the x cube edge. Here $K = 2\pi/\lambda$ is the wavevector and $\omega = 2\pi\nu$ is the angular frequency. If we substitute (58) into (57a) we find

$$\text{Longitudinal} \quad \omega^2 \rho = C_{11} K^2 ; \quad (59)$$

thus the velocity ω/K of a longitudinal wave in the [100] direction is

$$v_s = \nu\lambda = \omega/K = (C_{11}/\rho)^{1/2} . \quad (60)$$



Consider a transverse or shear wave with the wavevector along the x cube edge and with the particle displacement v in the y direction:

$$v = v_0 \exp [i(Kx - \omega t)] . \quad (61)$$

On substitution in (57b) this gives the dispersion relation

$$\omega^2 \rho = C_{44} K^2 ; \quad (62)$$

thus the velocity ω/K of a transverse wave in the $[100]$ direction is

$$\text{Transverse} \quad v_s = (C_{44}/\rho)^{1/2} . \quad (63)$$

The identical velocity is obtained if the particle displacement is in the z direction. Thus for \mathbf{K} parallel to $[100]$ the two independent shear waves have equal velocities. This is not true for \mathbf{K} in a general direction in the crystal.

Waves in the [110] Direction

There is a special interest in waves that propagate in a face diagonal direction of a cubic crystal, because the three elastic constants can be found simply from the three propagation velocities in this direction.

- (I) Consider a shear wave that propagates in the xy plane with particle displacement w in the z direction

$$w = w_0 \exp [i(K_x x + K_y y - \omega t)] , \quad (64)$$

whence (32c) gives

$$\omega^2 \rho = C_{44} (K_x^2 + K_y^2) = C_{44} K^2 , \quad (65)$$

Transverse

independent of propagation direction in the plane.

- (II) Consider other waves that propagate in the xy plane with particle motion in the xy plane: let

$$u = u_0 \exp [i(K_x x + K_y y - \omega t)] ; \quad v = v_0 \exp [i(K_x x + K_y y - \omega t)] . \quad (66)$$

From (57a) and (57b),

$$\begin{aligned} \omega^2 \rho u &= (C_{11} K_x^2 + C_{44} K_y^2) u + (C_{12} + C_{44}) K_x K_y v ; \\ \omega^2 \rho v &= (C_{11} K_y^2 + C_{44} K_x^2) v + (C_{12} + C_{44}) K_x K_y u . \end{aligned} \quad (67)$$

This pair of equations has a particularly simple solution for a wave in the [110] direction, for which $K_x = K_y = K/\sqrt{2}$. The condition for a solution is that the determinant of the coefficients of u and v in (67) should equal zero:

$$\begin{vmatrix} -\omega^2\rho + \frac{1}{2}(C_{11} + C_{44})K^2 & \frac{1}{2}(C_{12} + C_{44})K^2 \\ \frac{1}{2}(C_{12} + C_{44})K^2 & -\omega^2\rho + \frac{1}{2}(C_{11} + C_{44})K^2 \end{vmatrix} = 0 . \quad (68)$$

This equation has the roots

$$\omega^2\rho = \frac{1}{2}(C_{11} + C_{12} + 2C_{44})K^2 ; \quad \omega^2\rho = \frac{1}{2}(C_{11} - C_{12})K^2 . \quad (69)$$

The first root describes a longitudinal wave; the second root describes a shear wave. How do we determine the direction of particle displacement? The first root when substituted into the upper equation of (67) gives

$$\frac{1}{2}(C_{11} + C_{12} + 2C_{44})K^2 u = \frac{1}{2}(C_{11} + C_{44})K^2 u + \frac{1}{2}(C_{12} + C_{44})K^2 v , \quad (70)$$

Longitudinal

whence the displacement components satisfy $u = v$. Thus the particle displacement is along [110] and parallel to the \mathbf{K} vector (Fig. 20). The second root of (44) when substituted into the upper equation of (67) gives

$$\frac{1}{2}(C_{11} - C_{12})K^2 u = \frac{1}{2}(C_{11} + C_{44})K^2 u + \frac{1}{2}(C_{12} + C_{44})K^2 v , \quad (71)$$

Transverse

whence $u = -v$. The particle displacement is along $[1\bar{1}0]$ and perpendicular to the \mathbf{K} vector.

Selected values of the adiabatic elastic stiffness constants of cubic crystals at low temperatures and at room temperature are given in Table 11. Notice the general tendency for the elastic constants to decrease as the temperature is increased. Further values at room temperature alone are given in Table 12.

Table 11 Adiabatic elastic stiffness constants of cubic crystals at low temperature and at room temperature

The values given at 0 K were obtained by extrapolation of measurements carried out down to 4 K. The table was compiled with the assistance of Professor Charles S. Smith.

Crystal	Stiffness constants, in 10^{12} dyne/cm ² (10^{11} N/m ²)			Temperature, K	Density, g/cm ³
	C_{11}	C_{12}	C_{44}		
W	5.326	2.049	1.631	0	19.317
	5.233	2.045	1.607	300	—
Ta	2.663	1.582	0.874	0	16.696
	2.609	1.574	0.818	300	—
Cu	1.762	1.249	0.818	0	9.018
	1.684	1.214	0.754	300	—
Ag	1.315	0.973	0.511	0	10.635
	1.240	0.937	0.461	300	—
Au	2.016	1.697	0.454	0	19.488
	1.923	1.631	0.420	300	—
Al	1.143	0.619	0.316	0	2.733
	1.068	0.607	0.282	300	—
K	0.0416	0.0341	0.0286	4	
	0.0370	0.0314	0.0188	295	
Pb	0.555	0.454	0.194	0	11.599
	0.495	0.423	0.149	300	—
Ni	2.612	1.508	1.317	0	8.968
	2.508	1.500	1.235	300	—
Pd	2.341	1.761	0.712	0	12.132
	2.271	1.761	0.717	300	—

Table 12 Adiabatic elastic stiffness constants of several cubic crystals at room temperature or 300 K

	Stiffness constants, in 10^{12} dyne/cm ² or 10^{11} N/m ²		
	C_{11}	C_{12}	C_{44}
Diamond	10.76	1.25	5.76
Na	0.073	0.062	0.042
Li	0.135	0.114	0.088
Ge	1.285	0.483	0.680
Si	1.66	0.639	0.796
GaSb	0.885	0.404	0.433
InSb	0.672	0.367	0.302
MgO	2.86	0.87	1.48
NaCl	0.487	0.124	0.126

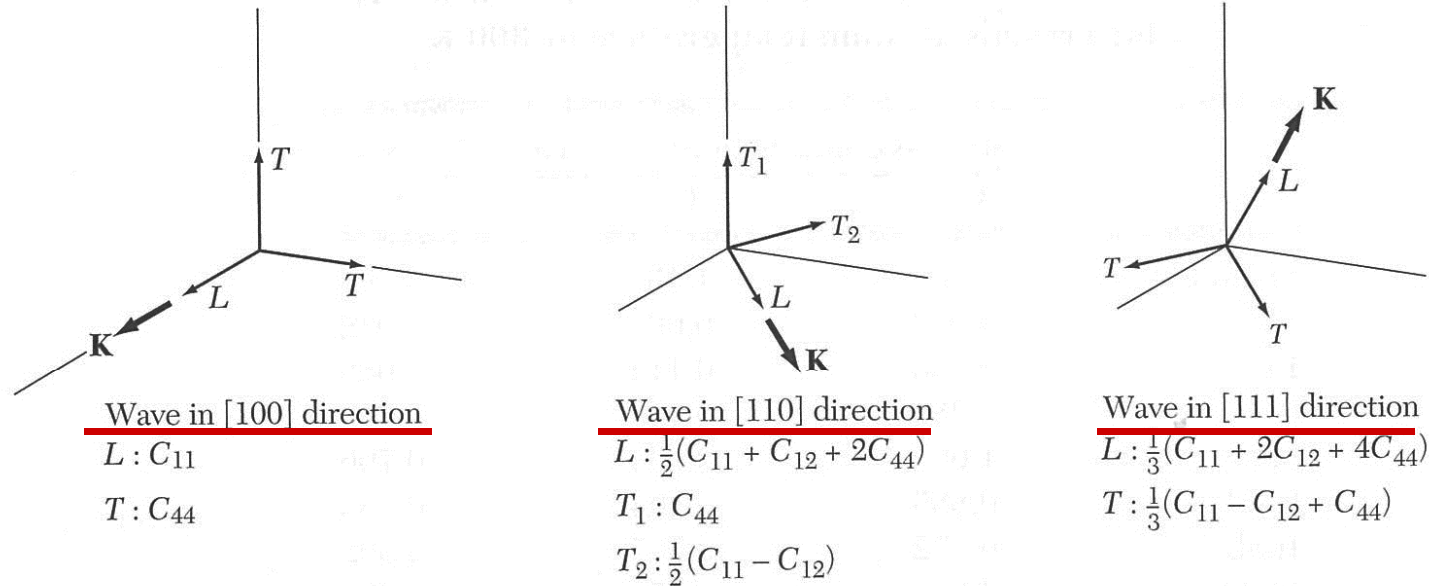
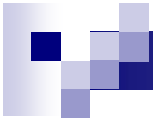


Figure 20 Effective elastic constants for the three modes of elastic waves in the principal propagation directions in cubic crystals. The two transverse modes are degenerate for propagation in the [100] and [111] directions.

There are three normal modes of wave motion in a crystal for a given magnitude and direction of the wavevector \mathbf{K} . In general, the polarizations (directions of particle displacement) of these modes are not exactly parallel or perpendicular to \mathbf{K} . In the special propagation directions [100], [111], and [110] of a cubic crystal two of the three modes for a given \mathbf{K} are such that the particle motion is exactly transverse to \mathbf{K} and in the third mode the motion is exactly longitudinal (parallel to \mathbf{K}). The analysis is much simpler in these special directions than in general directions.



The End of Chapter 3

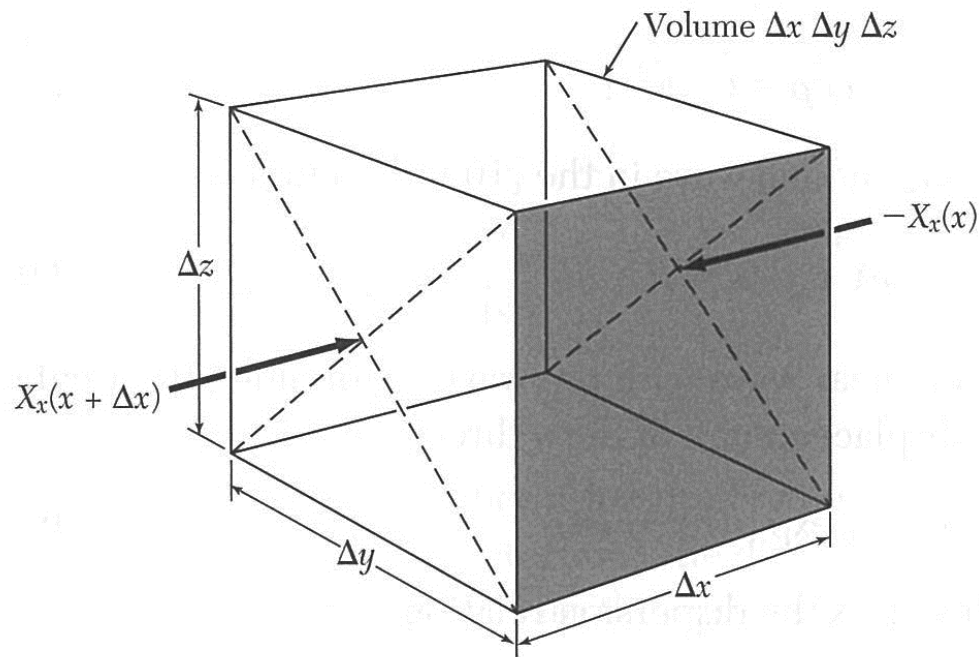


Figure 18 Cube of volume $\Delta x \Delta y \Delta z$ acted on by a stress $-X_x(x)$ on the face at x , and $X_x(x + \Delta x) \approx X_x(x) + \frac{\partial X_x}{\partial x} \Delta x$ on the parallel face at $x + \Delta x$. The net force is $\left(\frac{\partial X_x}{\partial x} \Delta x\right) \Delta y \Delta z$. Other forces in the x direction arise from the variation across the cube of the stresses X_y and X_z , which are not shown. The net x component of the force on the cube is

$$F_x = \left(\frac{\partial X_x}{\partial x} + \frac{\partial X_y}{\partial y} + \frac{\partial X_z}{\partial z} \right) \Delta x \Delta y \Delta z .$$

The force equals the mass of the cube times the component of the acceleration in the x direction. The mass is $\rho \Delta x \Delta y \Delta z$, and the acceleration is $\partial^2 u / \partial t^2$.

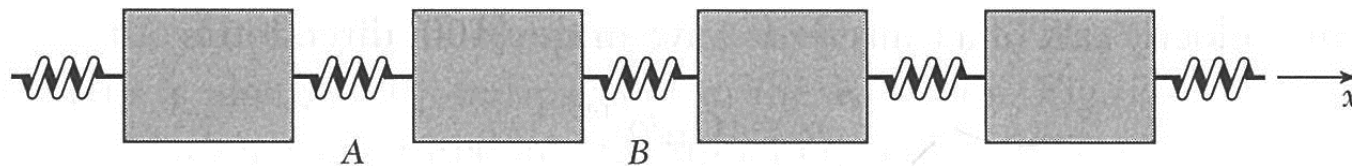


Figure 19 If springs A and B are stretched equally, the block between them experiences no net force. This illustrates the fact that a uniform stress X_x in a solid does not give a net force on a volume element. If the spring at B is stretched more than the spring at A , the block between them will be accelerated by the force $X_x(B) - X_x(A)$.

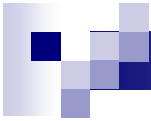


SUMMARY

- Crystals of inert gas atoms are bound by the van der Waals interaction (induced dipole-dipole interaction), and this varies with distance as $1/R^6$.
- The repulsive interaction between atoms arises generally from the electrostatic repulsion of overlapping charge distributions and the Pauli principle, which compels overlapping electrons of parallel spin to enter orbitals of higher energy.
- Ionic crystals are bound by the electrostatic attraction of charged ions of opposite sign. The electrostatic energy of a structure of $2N$ ions of charge $\pm q$ is

$$\text{(CGS)} \quad U = -N\alpha \frac{q^2}{R} = -N \sum \frac{(\pm)q^2}{r_{ij}} ,$$

where α is the Madelung constant and R is the distance between nearest neighbors.



- Metals are bound by the reduction in the kinetic energy of the valence electrons in the metal as compared with the free atom.
- A covalent bond is characterized by the overlap of charge distributions of antiparallel electron spin. The Pauli contribution to the repulsion is reduced for antiparallel spins, and this makes possible a greater degree of overlap. The overlapping electrons bind their associated ion cores by electrostatic attraction.