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Elastic Constant c_{44} of Uniaxial Layered Crystals

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For crystals with uniaxial layered structures the elastic constant c_{44} is given by a simple formula containing the frequency of a shear-type rigid-layer mode. The c_{44} of several layered compounds with already reported frequencies of these modes are calculated by this formula.

One of the most characteristic properties of lattice vibrations in crystals with layered structures is the existence of rigid-layer modes /1/. In most cases shear-type rigid-layer modes are Raman active. In this short note we report on the relation between the elastic constant c_{44} and the frequency of the shear-type rigid-layer mode. When Raman-active shear-type rigid-layer modes have been observed, we can estimate the approximate value of c_{44} .

In most layered crystals, the force between atoms in the same layer is known to be considerably larger than that between atoms in different layers. This allows us to apply a simple linear-chain model to deal with problems related to interlayer forces. Here we confine ourselves to the case of the vibration of the shear-type rigid-layer mode. The equation of motion of the n -th layer is expressed as

$$\rho d \frac{d^2 u_n}{dt^2} = f(u_{n+1} + u_{n-1} - 2u_n) \quad (1)$$

Here ρ is the density, d the distance between the center planes of the adjacent layers, f the force constant, u_n the displacement of the n -th layer. The solution of this equation for the mode corresponding to the maximum phase difference between the neighbouring layers is

$$f = \frac{\rho d}{4} \omega^2 \quad (2)$$

Here ω is the angular frequency of the mode. When the relative displacement of the adjacent layers is Δu , c_{44} is given by

$$c_{44} = \frac{f \Delta u}{\Delta u / d} \quad (3)$$

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The elastic constant c_{44} of uniaxial layered crystals at room temperature; d is the interplanar spacing, ω the angular frequency of the Raman-active shear-type rigid-layer mode, c_{44}^* the value calculated by (5) and c_{44}^{**} the value obtained by other methods

crystal	density (g cm ⁻³)	d (10 ⁻⁸ cm)	$\omega/2\pi c$ (cm ⁻¹)	c_{44}^* (GPa)	c_{44}^{**} (GPa)
2H-MoS ₂	5.000	6.147	33.7±1 /2/	19.0±1.1	18.6 /3/
2H-MoSe ₂	6.971	6.460	26.9 /4/	18.7	
			26.5 /5/	17.4	
2H-MoTe ₂	7.796	6.981	25.4 /4/	21.7	
			27.5 /5/	25.5	
2H-NbS ₂	4.63	5.94	31 /6/	13.9	
2H-NbSe ₂	6.44	6.27	30 /6/	20.2	19.0 /3/
2H-TaS ₂	7.07	6.05	26 /6/	15.5	
			27 /7/	16.7	
4Hb-TaS ₂			19 /8/	16.6	
2H-TaSe ₂	8.67	6.348	23 /6, 9/	16.4	
4Hb-TaSe ₂			16.5 /8/	16.9	
2H(β)-GaS	3.89	7.77	23.2 /10/	11.2	9.96±0.15 /11/ 9.5 /12/ 13.3 /13/
2H(ε)-GaSe	5.04	8.03	20.1±0.4 /14/	11.6±0.5	9.0±1 /11/ 10.0 /12/ 12.5 /13/
			19.7±1 /15/	11.2±1.1	
graphite	2.28	3.348	42 ±1 /16/	4.0±0.2	4.6 0.2 /17/ 4.0±0.4 /18/
hexagonal BN	2.28	3.331	52.5±1 /19/	6.2±0.2	

From (2) and (3) we obtain the relation

$$c_{44} = \frac{1}{4} \rho d^2 \omega^2 . \quad (4)$$

The mode which we refer here is Raman active in the layered crystals whose unit cells extend to more than one layer. Thus we can obtain the approximate value of c_{44} when the angular frequency of the Raman-active shear-type rigid-layer mode

has been measured. Usually the measurement of c_{44} requires samples of single crystals. The estimation of c_{44} by the above relation is based on the Raman data which even powder samples provide. Relation (4) holds when the phase difference between the adjacent layers is maximum and equal to π . When the phase difference is δ , the corresponding relation is

$$c_{44} = \frac{1}{4} \rho d^2 \omega^2 \left(\sin \frac{\delta}{2} \right)^{-2}. \quad (5)$$

We have calculated the values of c_{44} for several layered crystals according to (5). The results are summarized in Table 1. When the values of c_{44} have been obtained by other experimental methods, these values are shown in the last column for comparison. The values of c_{44} obtained by Raman data agree well to those obtained by the other experimental methods within an error of about 10%.

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