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Higher order elastic constants of rare earth metals : gadolinium, dysprosium and erbium

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Abstract. The expressions for the second and third order elastic constants of the rare earth metals, gadolinium dysprosium and erbium have been worked out and their values have been determined. The present theoretical values are compared with the experimentally observed results. It is also suggested that the third order elastic constants of these metals may be measured using ultrasonic technique under high pressures.

Keywords. Interlattice displacements; second order elastic constants ; third order elastic constants ; anharmonic parameters.

The rare earth metals gadolinium, dysprosium and erbium belong to the hexagonal close packed structure with c/a ratio equal to 1·590, 1·571 and 1·573 respectively. The second order elastic constants of these rare earths at various temperatures and pressures have been measured by Fisher *et al* (1973). The expressions for the second order and third order elastic constants are worked out under the quasiharmonic approximation for the hexagonal metals. The physical significance of the different parameters used are given by Menon and Rao (1972).

The basic vectors of the lattice are

$$\vec{a}_1 = D\,(\tfrac{1}{2}\sqrt{3}, \tfrac{1}{2}, 0),$$

$$\vec{a}_2 = D\,(0, 1, 0),$$

$$\vec{a}_3 = D\,(0, 0, P),$$

referred to the cartesian system of axes, D is the nearest neighbour in the basal plane and P is the axial c/a ratio. These are two nonequivalent atoms in the unit cell at $r\,(1) = D\,(0, 0, 0)$ and $\vec{r}_2 = D\,(\tfrac{1}{2}\sqrt{3}, \tfrac{1}{2}, \tfrac{1}{2}P)$. The atom 1 in the basic cell has three sets of neighbours of the same type and three other sets of the non-equivalent type.

Table 1. Second order elastic constants of gadolinium, dysprosium and erbium in 10^{11} dyn/cm^2. Experimental values are those of Fisher *et al* (1973).

Rare-earth metal	C_{11}		C_{12}		C_{13}		C_{33}		C_{44}		C_{66}	
	Present work	Experimental	Present work	Experimental	Present work	Experimental	Present work	Experimental	Present work	Experimental	Present work	Experimental
Gd	6·67	6·67	2·50	2·50	2·13	2·13	7·19	7·19	2·07	2·07	2·08	2·08
Dy	7·47	7·47	2·62	2·62	2·23	2·23	7·87	7·87	2·31	2·43	2·43	2·43
Er	8·63	8·63	3·05	3·05	2·27	2·27	8·54	8·55	2·81	2·81	2·79	2·79

Table 2. Third order elastic constants of gadolinium, dysprosium and erbium in 10^{11} dyn/cm^2.

Rare-earth metal	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{144}	C_{155}	C_{222}	C_{333}	C_{344}
Gd	−50·3	−13·3	+0·4	−6·3	− 9·7	−3·9	−2·0	−55·1	−76·2	− 9·7
Dy	−53·2	−16·4	−0·8	−6·9	−12·4	−4·6	−3·1	−62·0	−73·5	−12·4
Er	−79·6	−18·7	−5·0	−7·0	−16·7	−5·4	−6·6	−87·8	−74·7	−16·7

In a homogeneous deformation, the components of the interatomic vectors are altered as follows :

$$R_i'\begin{pmatrix} L\,L' \\ \mu\,\mu' \end{pmatrix} = R_i\begin{pmatrix} L\,L' \\ \mu\,\mu' \end{pmatrix} + \sum_j \epsilon_{ij}\, R_j\begin{pmatrix} L\,L' \\ \mu\,\mu' \end{pmatrix} + W_i(1 - \delta\mu\mu').$$

Here $R_i\begin{pmatrix} L\,L' \\ \mu\,\mu' \end{pmatrix}$ is the vector distance between the particle μ in the cell L and the particle μ' in the cell L' in the unstrained state. $R_i'\begin{pmatrix} L\,L' \\ \mu\,\mu' \end{pmatrix}$ refers to the vector distance in the homogeneously deformed state. ϵ_{ij} is the deformation parameter related to the macroscopic Lagrangian strains by

$$\eta_{ij} = \tfrac{1}{2}\left[\epsilon_{ij} + \epsilon_{ji} + \sum_k \epsilon_{ik}\epsilon_{jk}\right]$$

and W_i is the component of the internal displacement of the sublattice $\mu = 2$ relative to $\mu = 1$. The internal displacement components are replaced by

$$\bar{W}_i = W_i + \sum_j \epsilon_{ji} W_j.$$

In terms of η_{ij} and $\bar{W}_i$ the energy is invariant towards rigid rotations of the crystal. $\bar{W}_i$ can be obtained in terms of η_{ij} to the first order by minimising the strain energy with respect to $\bar{W}_i$. The large number of second order and third order anharmonic parameters are not elaborated in this paper. Instead, we enumerate the results obtained in each case. Table 1 gives the values of the second order elastic constants calculated along with the experimental values. The agreement is quite good. However as no experiment has been carried out to obtain the third elastic constants of these metals, only the theoretical values are reported in table 2. It is desirable to determine the complete set of third order elastic constants of these rare earth materials using the ultrasonic wave velocity measurements under high pressures. At present the other anharmonic properties like the thermal conductivity are being investigated in this laboratory.

References

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