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## Third-order elastic constants and pressure derivatives of erbium.

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The ten third-order elastic (TOE) constants of erbium have been calculated from a nearest-neighbour central-interaction model. The calculated TOE constants are used to evaluate the pressure derivatives of the second-order elastic (SOE) constants of erbium and are compared with the measured values. The TOE constants of erbium obtained on the central-force model agree well with those obtained from Keating's model for hexagonal metals.

In this paper the third-order elastic (TOE) constants of erbium have been evaluated using the nearest-neighbour central-force model (C.F. model) of Ramji Rao & Srinivasan (1968) for ideal h.c.p. structures. The calculated TOE constants are then used to evaluate the pressure derivatives of the second-order elastic (SOE) constants of erbium which are compared with the measured values of Fisher, Manghnani & Kikuta (1973).

The expressions for the SOE and TOE constants of an ideal h.c.p. lattice were derived by Ramji Rao & Srinivasan (1968) who used a nearest-neighbour central-interaction potential of the form

$$\Phi(r) = -\frac{a}{r^m} + \frac{b}{r^n} . \qquad (1)$$

These expressions involve two constants $k_2$ and $k_3$:

$$k_2 = (\mathrm{O}'^2\Phi) \quad = \frac{\eta M}{2D^2}$$

and

$$k_3 = (\mathrm{O}'^3\Phi) \quad = -\frac{\eta}{4}\frac{M}{D^4}(n+m+6) . \qquad (2)$$

Here $M$ is the mass of the atom and

$$\eta = \frac{n(n-m)b}{2MD^{n+2}} . \qquad (3)$$

O′ is the differential operator $\partial/\partial(r^2)$.

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Srinivasan & Ramji Rao (1965) showed that the high-temperature limit of the Grüneisen parameter of an ideal h.c.p. lattice described by the nearest-neighbour central potential is nearly equal to $(n+m)/6$. Gschneidner (1964) reports a value of 1.17 for the thermal $\bar{\gamma}_H$ of erbium. So the value of $(n+m)$ appropriate to erbium is seven. In order to calculate the TOE constants, we need to know the value of $\eta$ for erbium. The measured SOE constants $C_{11}$ and $C_{33}$ of Fisher *et al.* (1973) and $D = 3.562$ A.U. are used to get an average value of $\eta$. Hence $k_2$ and $k_3$ are evaluated. The expressions for the effective SOE constants $C'_{IJ}$ of a strained hexagonal crystal in terms of its TOE constants were derived by Ramji Rao & Srinivasan (1969) using the finite strain theory of Murmaghan (1951). The pressure derivatives of erbium can be obtained by differentiating $C^1_{IJ}$ with respect to the pressure $p$ and using the calculated values of the TOE constants. Finally these are compared with the measured values of Fisher *et al.* (1973). The present calculated TOE constants and pressure derivatives of erbium based on the nearest-neighbour C.F. model are compared with those obtained by Ramji Rao & Menon (1973) from the theory of hexagonal metals developed by Srinivasan & Ramji Rao (1971) on the basis of Keating's (1966) approach. The calculated TOE constants and pressure derivatives from the C.F. model and those from the Keating's model together with the experimental pressure derivatives are given in Table 1.

From Table 1, we find that there is good agreement between the two sets of the TOE constants of erbium calculated from the two models. The pressure derivatives $dC_{33}/dp$ and $dC_{66}/dp$ of the C.F. model deviate from the

Table 1. *TOE constants and pressure derivatives of erbium from the central-force model and comparison with those from Keating's model*

| | TOE constants in $10^{11}$dynes/cm$^2$ | | | Pressure derivatives | | Measured value at room temperature |
|---|---|---|---|---|---|---|
| $C_{IJK}$ | from C.F. model | from Keating's model | $\frac{dC_{IJ}}{dp}$ | from C.F. model | from Keating's model | |
| $C_{111}$ | −74·7 | −79·6 | | | | |
| $C_{222}$ | −91·2 | −87·8 | $\frac{dC_{11}}{dp}$ | 4·82 | 4·77 | 4·77 |
| $C_{333}$ | −78·3 | −74·7 | | | | |
| $C_{112}$ | −25·7 | −18·7 | $\frac{dC_{33}}{dp}$ | 6·14 | 5·45 | 5·45 |
| $C_{113}$ | −3·8 | −5·0 | | | | |
| $C_{123}$ | −6·0 | −7·0 | $\frac{dC_{44}}{dp}$ | 1·03 | 0·95 | 0·95 |
| $C_{133}$ | −19·6 | −16·7 | | | | |
| $C_{144}$ | −4·9 | −5·4 | $\frac{dC_{66}}{dp}$ | 1·04 | 0·85 | 0·85 |
| $C_{155}$ | −4·9 | −6·6 | | | | |
| $C_{344}$ | −19·6 | −16·7 | $\frac{dC_{12}}{dp}$ | 2·74 | 3·06 | 3·06 |
| | | | $\frac{dC_{13}}{dp}$ | 2·07 | 2·00 | 2·16 |

measured values by 11 and 18% respectively. The expressions for the TOE constants on the Keating model involve the anharmonic stretching force constants $\nu$ and $\chi$ of the $M$ and $K$ atoms respectively. The $M$ atoms are the second non-equivalent neighbours out of the basal plane and the $K$ atoms are the third-equivalent neighbours along the $c$ axis. In the nearest-neighbour C.F. model the interactions of $I$ and $J$ atoms only are involved. Thus the limitation on the C.F. model is its short-range central interaction due to which the agreement between the calculated and the experimental pressure derivatives of $C_{33}$ and $C_{66}$ is not good. $dC_{33}/dp$ and $dC_{66}/dp$ involve the farther-neighbour interactions of $K$ and $M$ atoms. Also we find that the bending force constant $\varepsilon$ of the $J$ atoms has a minor role in the evaluation of the TOE constants of erbium. It would be appropriate to mention here that the $(m+n)$ value of erbium has a low value of seven, which is a consequence of the simple power law assumed in the C.F. model. However, the C.F. model brings out clearly the fact that central forces are predominant in this rare-earth metal erbium. The straight constants $C_{111}$, $C_{222}$ and $C_{333}$ are nearly the same (in both the models) indicating elastic isotropy for this metal.

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## References

FISHER, E. S., MANGHNANI, M. H. & KIKUTA, R. (1973). *J. Phys. Chem. Solids*, **34**, 687–703.

GSCHNEIDNER, K. A JR (1964). *Solid State Phys.* **16**, 414.

KEATING, P. N. (1966). *Phys. Rev.* **145**, 637–645.

KEATING, P. N. (1966). *Phys. Rev.* **149**, 674–678.

MURMAGHAN, F. D. (1951). *Finite Deformation of an Elastic Solid.* New York: John Wiley.

RAMJI RAO, R. & MENON, C. S. (1973). *J. Appl. Phys.* **44**, 3892–3896.

RAMJI RAO, R. & SRINIVASAN, R. (1968). *Phys. Stat. Sol.* **29**, 865–871.

RAMJI RAO, R. & SRINIVASAN, R. (1969). *Phys. Stat. Sol.* **31**, K39–K42.

SRINIVASAN, R. & RAMJI RAO, R. (1965). *Inelastic Scattering of Neutrons*, **1**, pp. 325–342. Vienna: IAEA.

SRINIVASAN, R. & RAMJI RAO, R. (1971). *J. Phys. Chem. Solids*, **32**, 1769–1788.