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Note

Fourth-Order Elastic Constants of β-Brass

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Combinations of the fourth-order elastic constants of β-brass were calculated using the measured second-order and third-order elastic constants and the expressions for the effective elastic constants of a cubic crystal obtained from finite-strain theory. The present calculations show that the Cauchy relations for the fourth-order elastic constants in β-brass are not satisfied. This implies that noncentral or many-body forces occur in this material. We consider two alloys. The higher-Zn alloy shows lower magnitudes of the fourth-order elastic constants and a larger Cauchy discrepancy.

KEY WORDS: anharmonicity; β-brass; Cauchy relationships; elastic constants.

1. INTRODUCTION

Higher-order elastic constants are extremely useful in studying the anharmonic properties of solids. Third-order and fourth-order elastic constants (TOECs and FOECs, respectively) are necessary to evaluate the third-order and fourth-order terms of the potential energy of a solid, and they directly measure a material's anharmonicity. These higher-order elastic constants are important in the calculation of many anharmonic effects, examples of which are the generalized Grüneisen parameters, which describe the strain dependence of the lattice-vibrational frequencies, the

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pressure and temperature dependence of the second-order elastic constants, the thermal relaxation of sound waves at high frequencies, and the specific heat at high temperatures.

2. THEORY

In this study, we calculated combinations of the FOECs of β-brass for two compositions. The SOECs and TOECs and the first pressure derivatives of β-brass of two compositions—44.3 at% Zn and 48.3 at% Zn—were measured by Swartz et al. [1]. The present calculations used numbers given in Tables I, III, and IV of Ref. 1. Ramji Rao and Padmaja [2] obtained expressions for the effective SOECs of a cubic crystal to the second degree in the Lagrangian strains in terms of its natural SOECs, TOECs, and FOECs using the finite-strain theory of Murnaghan [3]. For convenience, these expressions are given here.

$$\begin{aligned} C^{1}_{11} = {} & C_{11} + \eta(3C_{11} + 4C_{12} + C_{111} + 2C_{112}) \\ & + \eta^2(-5/2\, C_{11} - 4C_{12} + 2C_{111} + 8C_{112} + 2C_{123} \\ & + 1/2\, C_{1111} + 2C_{1112} + C_{1122} + C_{1123}) \end{aligned} \tag{1}$$

$$\begin{aligned} C^{1}_{12} = {} & C_{12} + \eta(C_{12} + 2C_{112} + C_{123}) \\ & + \eta^2(-1/2\, C_{12} + 2C_{112} + C_{123} + C_{1112} + C_{1122} + 5/2\, C_{1123}) \end{aligned} \tag{2}$$

$$\begin{aligned} C^{1}_{44} = {} & C_{44} + \eta(C_{11} + 2C_{12} + C_{44} + C_{144} + 2C_{155}) \\ & + \eta^2(-C_{11} - 2C_{12} - 1/2\, C_{44} + 1/2\, C_{111} + 3C_{112} + C_{123} \\ & + C_{144} + 2C_{155} + 1/2\, C_{1144} + C_{1155} + 2C_{1255} + C_{1266}) \end{aligned} \tag{3}$$

Here η denotes the Lagrangian strain given by $\eta = \varepsilon/3$, and ε denotes the uniform volume strain under a hydrostatic pressure, p. Thus,

$$\eta = \frac{-p}{(C_{11} + 2C_{12})} \tag{4}$$

Results of FOEC combinations obtained from these expressions appear in Table I.

Table I. Combinations of FOECs for β-Brass in Units of TPa

Combinations of FOECs	44.3 at% Zn	48.3 at% Zn
$\gamma^{(4)}_{11} = C_{1111} + 4C_{1112} + 2C_{1122} + 2C_{1123}$	30.706	27.222
$\gamma^{(4)}_{12} = 2C_{1112} + 2C_{1122} + 5C_{1123}$	16.471	14.111
$\gamma^{(4)}_{44} = C_{1144} + 2C_{1155} + 4C_{1255} + 2C_{1266}$.	10.471	8.222

3. DISCUSSION

All the TOECs of β-brass are negative, and the combinations of its FOECs, as expected, are all positive. The order of magnitude of the TOECs is about 10 times that of the SOECs, and the FOECs about 100 times that of the SOECs. This shows the slow convergence of the Taylor expansion of the internal energy with respect to the Lagrangian strains. Validity of the Cauchy relations for the FOECs requires that $\gamma_{12}^{(4)} = \gamma_{44}^{(4)}$ [4], and this is not satisfied, as shown in Table I. This implies that in β-brass, which has a CsCl crystal structure, the short-range repulsive forces are not purely central, that neighbor interactions extend beyond second neighbors, and that three-body interactions may have to be considered to evaluate its FOECs. Swartz et al. [1] estimated the FOECs of β-brass using a short-range central potential of the Born–Mayer type and considering only nearest-neighbor (n-n) and next-nearest-neighbor (n-n-n) interactions. This enabled them to use the relationships

$$C_{1112} = C_{1122} = C_{1123} \tag{5}$$

Together with the Cauchy conditions, these reduce the 11 FOECs to only 2. However, in view of the present calculations, these assumptions of Swartz et al. do not hold for β-brass. Perhaps the use of an anharmonic potential of the Keating type [5] would remove the degeneracy among its FOECs. For the two alloys considered, the one with the higher Zn content showed lower magnitudes of the FOEC combinations and a larger Cauchy discrepancy. Since experimental TOECs and first pressure derivatives of the SOECs of β-brass have been used to evaluate its FOEC combinations, one expects the present values to be nearer to the actual values.

4. CONCLUSIONS

From this study, we reach the following conclusions.

(1) The Cauchy relations for the FOECs are not valid in β-brass.

(2) Noncentral and many-body interactions should be considered for the evaluation of the FOECs of β-brass. Relationship (5) does not hold.

(3) The higher-Zn alloy shows lower magnitudes of the FOECs.

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