

THE PRESSURE COEFFICIENT OF THE SHEAR MODULUS OF V_3Si^*

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ABSTRACT

The temperature dependence of the pressure coefficient of the shear modulus $c_s = (c_{11} - c_{12})/2$ has been calculated from the linear chain model by including interband charge transfer under pressure. For a suitable choice of the charge transfer parameter it is possible to obtain semiquantitative agreement with the experimental data for transforming V_3Si , but not for nontransforming V_3Si . This suggests that transforming crystals correspond more closely to the ideal of the linear chain model, and that the quantitatively and qualitatively different behavior of nontransforming crystals arises from crystal imperfections.

Introduction

An anomalous softening of the elastic shear modulus $c_s = (c_{11} - c_{12})/2$ is known to occur for some Al5-structure intermetallic compounds with high superconducting transition temperatures (1-5), including V_3Si (1,3). Closely related to this elastic softening is a martensitic-like structural transformation from the cubic to the tetragonal phase. For V_3Si this transformation is observed between about 18 and 25°K (1,6,7).

The structural transformation does not occur in all samples of a given Al5 compound, and different parts of the same crystal boule may show different behavior. The cause of this is still unknown (7,8). It has been reported that specimens from the seed end of a boule show a tendency not to transform, whereas sections of the boule farther away from the seed end usually undergo the transformation (7,8). The different behavior has been tentatively attributed to the

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presence of heterophase inclusions in transforming crystals (7-10), but the microscopically visible amount of second phase (presumably V_5Si_3 or V (9,11)) did not correlate with the tendency to transform, whereas the electrical resistance ratio R_{300}/R_{20} was found to be a relevant measure (7,8). The resistance ratios of nontransforming specimens are usually low (about 10), and those of transforming specimens high (up to about 80) (7,8). It has further been observed that nontransforming crystals of Nb_3Sn became transforming after heat treatment (8,12).

The difference between transforming and nontransforming crystals is also apparent in their elastic behavior. Transforming samples show a stronger softening and smaller values of the shear modulus c_s than nontransforming samples (3), and the temperature dependence of the pressure coefficient ($\partial c_s / \partial p$) is quantitatively and qualitatively different for the two types of samples (13-15).

It is the purpose of the present paper to calculate the temperature dependence of ($\partial c_s / \partial p$) for V_3Si on the basis of the linear chain model of Labbé and Friedel (16). The results shed some new light on the possible explanations for the different behavior and suggest that for V_3Si transforming samples are structurally more perfect than nontransforming samples.

The variation of ($\partial c_s / \partial p$) with temperature has been calculated before by Schuster (17) from the electron-renormalized sound velocity (18) based on the one-dimensional electronic density of states of Labbé and Friedel (16). As has been noted before, the theoretical curve agrees between 77°K and 300°K approximately with the experimental data (13-15), but at lower temperatures it cannot account for the behavior of either transforming or nontransforming V_3Si (14). It will be shown below that the discrepancy arises from the fact that in Schuster's treatment the electronic charge transfer between the d-band and the s-band is neglected, and that inclusion of the charge transfer* results in good semiquantitative agreement with the experimental data for transforming V_3Si .

Calculation of ($\partial c_s / \partial p$)

The expression for the electron-renormalized sound velocity used by Schuster (17) is equivalent to the expression derived by Barišić and Labbé (19) on the

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