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Title
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Permalink
https://escholarship.org/uc/item/2cv7222h

Journal
Physics Letters A, 53(1)

ISSN
0375-9601

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Publication Date
1975-05-01

DOI
10.1016/0375-9601(75)90336-9

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Peer reviewed

ISOTOPE EFFECT IN THE RESISTIVITY OF SCANDIUM HYDRIDE [☆]

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The temperature dependent resistivities of ScH_2 and ScD_2 differ by an Einstein term with $\theta_E = 1600$ K and $\theta_E/\sqrt{2}$, respectively.

Heat capacity measurements [1, 2] have shown that the phonon spectra of YH_2 and ZrH_2 contain high frequency Einstein modes due to the presence of H in these compounds. Substitution of D for H resulted in a decrease in the Einstein temperature by $\sqrt{2}$, with corresponding changes in the temperature dependence of the heat capacity. We suspected that electron scattering from these Einstein modes would also be evident in the electrical resistivities of transition metal hydrides. We chose to work with the isoelectronic, iso-structural pair ScH_2 and ScD_2, since they are easily prepared [3] and there are no competing higher hydrides of Sc [3, 4].

Solid pieces of Sc (99.9%) were reacted with hydrogen (UHP) or deuterium (99.5%) at a pressure of one atm at 600°C for several hours. The temperature was then lowered to room temperature over a period of 12 hours. Gravimetric analysis of representative samples of the hydride indicated a stoichiometry of the final products given by $ScH_{1.98\pm0.02}$. X-ray analysis of ScH_2 showed a face-centered-cubic lattice with lattice parameter 4.783 ± 0.001 Å, in excellent agreement with previous determinations [3, 4]. Apart from two very weak extra lines in the X-ray patterns which indicate the presence of a few percent of Sc_2O_3 in the samples, all diffraction lines were due to ScH_2.

The resistivities of our samples of ScH_2 and ScD_2 showed very small resistance minima near 4 K which were probably due to trace magnetic impurities in the Sc. No superconductivity was observed above 2 K for either sample. Between 15 and 100 K, the resistivities for both samples followed the Bloch-Grüneisen theory [e.g. 5]: $R(T) = 4\mathcal{R}(T/\theta_R)^5 \mathcal{J}_5(\theta_R/T)$, where $\mathcal{R}$ is a constant, θ_R is the resistivity Debye temperature, and $\mathcal{J}_5(x)$ is the transport integral of order 5. Fitting the data to this theory, we obtain $\theta_R = 490$ K for both samples. $\mathcal{R}$ was also determined (see below). However, above 100 K, the temperature dependent resistivities of ScH_2 and ScD_2 diverge both from this theory and from each other. The latter divergence is illustrated in the inset of fig. 1, where the measured resistance of ScH_2 is plotted versus the resistance of ScD_2.
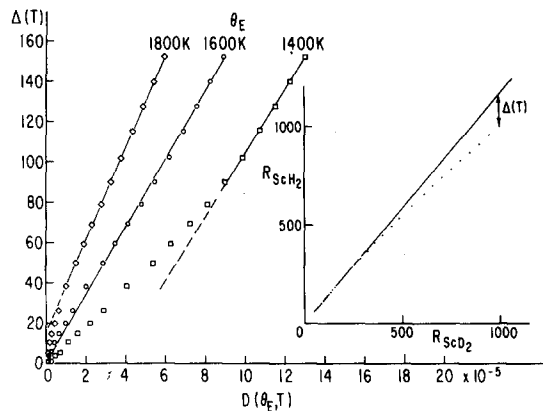

Fig. 1. Inset: Resistance of ScH_2 plotted versus the resistance of ScD_2 (in arbitrary units), over the temperature range 15 to 290 K. The deviation $\Delta(T)$ of the data from the straight line is attributed to electron scattering from H and D Einstein modes with Einstein temperatures θ_E and $\theta_E\sqrt{2}$, respectively. To the left of the inset, the deviation $\Delta(T)$ is plotted versus a theoretical optical mode scattering expression $D(\theta_E, T)$ for several values of θ_E, yielding $\theta_E = 1600$ K.

The data lie on a straight line for temperatures below 100 K, since in this temperature range the temperature dependent resistivities are identical: $R_{ScH_2} = A + BR_{ScD_2}$ ($15\,K \lesssim T \lesssim 100\,K$). Above 100 K, however, $R_{ScH_2} = A + BR_{ScD_2} + \Delta(T)$, where $\Delta(T)$ is a function of temperature to be discussed below.

In order to analyze the temperature dependent deviation $\Delta(T)$, we assume that the only difference in the temperature dependent resistivities of ScH_2 and ScD_2 is due to conduction electron scattering by Einstein modes whose Einstein temperatures are θ_E and $\theta_E/\sqrt{2}$ in the respective compounds [1, 2]. Howarth and Sondheimer showed [6] that to lowest order, the resistance due to scattering by an Einstein mode is proportional to $E(\theta_E, T)/M$, where M is the mass of the atoms responsible for the Einstein mode, and $E(\theta_E, T)$ is a function given by $E(\theta_E, T) = (T \sinh^2 \times (\theta_E/2T))^{-1}$. Therefore, if our model is correct, we have

$$\Delta(T) \propto \left[\frac{E(\theta_E/\sqrt{2}, T)}{2} - E(\theta_E, T) \right] \equiv D(\theta_E, T). \quad (1)$$

In fig. 1, we have plotted $\Delta(T)$ versus $D(\theta_E, T)$ for $\theta_E = 1400\,K$, $1600\,K$, and $1800\,K$. Comparing eq. (1) with the data in fig. 2 yields $\theta_E = 1600 \pm 100\,K$. The constant of proportionality in eq. (1) can also be determined from the slope of the plot for $\theta_E = 1600\,K$, thereby completely specifying the Einstein mode scattering versus temperature (in our arbitrary units). Our value of θ_E is in good agreement with the Einstein temperatures of 1700 K [1] and 1500 K [2] found from heat capacity measurements for the similar compounds ZrH_2 and YH_2, respectively.

The relative scattering cross section of acoustic to optical modes can be obtained from the high temperature limit ($T \gg \theta_R$, $T \gg \theta_E$) where the atoms in the compound scatter independently. Using the asymptotic forms of the Bloch-Grüneisen and Einstein terms, we have in our arbitrary units the following high temperature limit (normalized to the same atomic vibration amplitude $T/M\theta^2$):

$$R_{ScH_2} = R_{Bloch\text{-}Gr\ddot{u}neisen} + R_{Einstein}$$

$$= 42.6\,\frac{T}{M_{ScH_2}\theta_R^2} + 6.7\,\frac{T}{M_H\theta_E^2}.$$

The first term represents the acoustic mode scattering in which we suppose the hydrogen atoms to follow rigidly the Sc motion, and the second term the Einstein contribution from both hydrogen atoms. A more specific model would be required to further compare the relative Sc and H scattering cross sections. We note, however, that the ratio of the two coefficients (6.4) is in rough agreement with the simple estimate obtained by assuming +3 and +1 charges on the Sc and H, respectively, and additivity of cross sections of Sc and H in the acoustic mode scattering; i.e., (9+2)/2 = 5.5.

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