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Elastic properties of MnSi, FeSi and CoSi

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Abstract. Measurements of sound velocities in single crystals of MnSi, FeSi and CoSi were performed in the temperature range 2.5-300 K and elastic constants were calculated. The temperature dependence of the elastic constants reveal nontrivial features, reflecting specifics of the magnetic and electronic subsystems in these materials.

The intermetallic compounds MnSi, FeSi and CoSi with a cubic B20 crystal structure have attracted much attention over decades due to their remarkable magnetic and electrical properties. MnSi is an itinerant helical magnet with a Curie point of 29 K. FeSi, a strongly correlated semiconductor, having a small energy gap of about 0.05 eV at low temperature, reveals metallic properties above 100 K [1, 2, 3, 4, 5]. CoSi is a semimetal with very high residual resistivity, implying existence of a fairly large number of defects [6]. Although these compounds display a range of properties their lattice parameters change very little consistent with the trend in metallic radii for Mn, Fe and Co. Together these facts tell us that the total energies of these systems are not sensitive to the details of their electronic and magnetic structures. However, as is shown below the specifics of the macro properties of these silicides can be observed through the second derivatives of the total energy with respect to deformation, i.e. their elastic properties.

We report here results of ultrasonic studies of single crystals of MnSi, FeSi and CoSi. The measurements were performed using a digital pulse-echo technique (see details in Ref. [7]) in the temperature range 4-300 K (4-150 K for MnSi). The single crystals were grown by the Bridgman (MnSi, CoSi) and the Czokhralski (FeSi) methods. The lattice parameters of the crystals, determined by X-ray diffraction, correspond well to literature values (see Table. 1). For the ultrasonic studies, samples of MnSi, FeSi and CoSi of about 2 - 4 mm thicknesses and with orientations along [100], [110] and [111] were cut from big single crystals. The corresponding surfaces of the samples were made optically flat and parallel. The 36° Y (P-wave) and 41° X (S-wave) cut $LiNbO_3$ transducers were bonded to the samples with various adhesives, including silicon greases and super glue. Temperature was measured by a calibrated Cernox sensor with an accuracy of 0.02 K. The speed of sound and elastic constants are calculated using the known thickness and density of the samples and the relationship $c_{ij} = \rho V^2$. The precision of the sound velocity measurements is about 0.1%, though the absolute accuracy may be of order 1% mainly due to uncertainty connected with a phase shift at the transducers sample bond interface. Results of the measurements and calculations are shown in Figures 1 to 6 and Table 1. Some our data for MnSi have been already published in Ref. [7]. They are partly reproduced here for the comparison purpose. Low resolution ultrasonic data for a number of transition metal silicides were published in [8]. The temperature dependence of the elastic moduli of FeSi was measured

previously using the resonant ultrasound spectroscopy technique [9]. The data from Ref. [9] generally agrees with our results, where they overlap at temperatures ($T > 77K$), although slight differences in temperature calibration are present.

Now we turn to the analysis of the current experimental data. As is seen from Figures 1- 3, the numerical values of the elastic constants in the row MnSi-FeSi-CoSi change according to positions of the metallic atoms in the Mendeleev periodic table or, in the other words, according to the number of 3d valence electrons in these compounds. A slight difference in this characteristic of the compounds evidently results in subtle variation of the cohesion energies and lattice parameters, that caused quite an observable difference in the elastic constants (see Figures 1- 4). It needs to be emphasized that regularity in the variation of the elastic constants variation exist despite the specifics electronic and magnetic structures of the compounds. Indeed it is instructive to look at the situation at low temperatures where CoSi is a semimetal with a good metallic value of the Sommerfeld constant $\gamma = 1.1mJ/moleK^2$ [10], FeSi is a narrow gap semiconductor, and MnSi is a metal with helical magnetic structure and a very large $\gamma = 36mJ/moleK^2$ [11]. The values of c_{11} and c_{12} elastic constants are highest for CoSi, then follow FeSi and MnSi (Fig. 1, 2). The situation is different in case of the shear elastic constant c_{44} (Fig. 3) where FeSi has now the highest value, and CoSi the smallest.

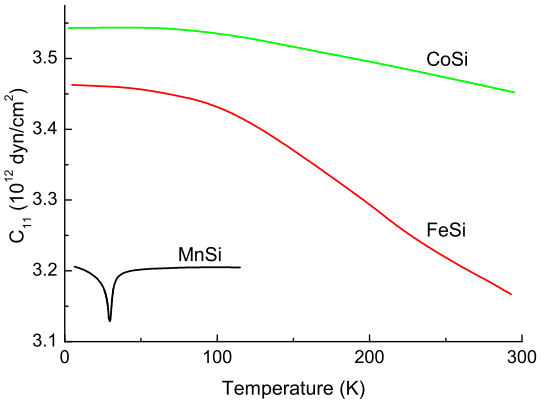

Figure 1. (Color online) Elastic constants c_{11} of MnSi, FeSi and CoSi

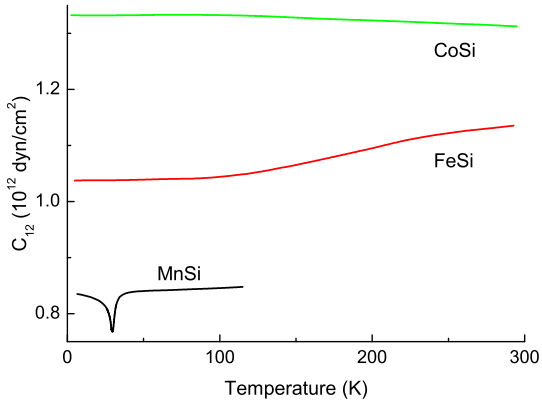

Figure 2. (Color online) Elastic constants c_{12} of MnSi, FeSi and CoSi

It seems quite natural that CoSi with the highest electron concentration, has the highest bulk modulus $K = (c_{11} + 2c_{12})/3$. At the same time, it is not quite clear why CoSi should have the smallest shear moduli c_{44} and $(c_{11} - c_{12})/2$.

The temperature variations of the elastic properties of the three compounds are far from triviality. Though in the case of CoSi there are no significant features to be seen on the scale of Figs. 1- 3. However, if we look closely at the temperature dependence of CoSi below 60 K Fig. 5, we can clearly see an unusual softening of the elastic constants. The elastic constants c_{11} and c_{44} of FeSi strongly decrease at high temperature as compared with CoSi; whereas, c_{12} grows anomalously over the entire range of temperature. As a consequence the shear module $(c_{11} - c_{12})/2$ of FeSi drops off precipitously above 100 K (Fig. 4). This behavior is consistent with the gap closing as indicated in [12, 13]. The MnSi elastic constants that control propagation of longitudinal waves reveal significant softening at $\sim$ 30 K and small discontinuities at 28.8 K, which corresponds to the magnetic phase transition in MnSi. In contrast, the shear elastic moduli, do not show any softening at all and only respond to small volume deformations caused by the magneto-volume effect [11].

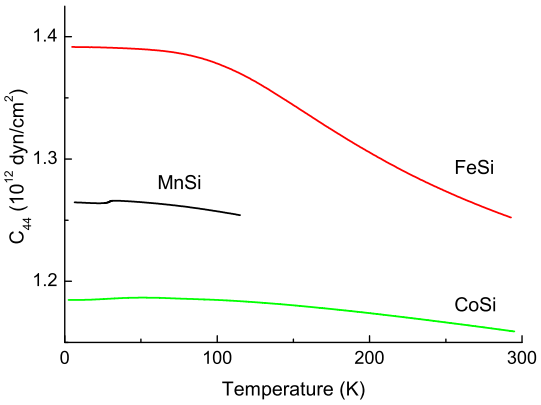

Figure 3. (Color online) Elastic constants c_{44} of MnSi, FeSi and CoSi

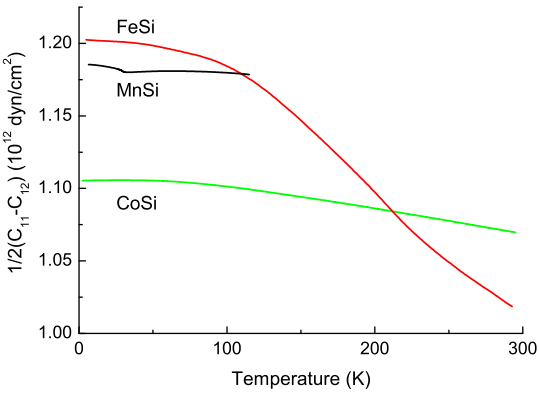

Figure 4. (Color online) Shear moduli $(c_{11} - c_{12})/2$ of MnSi, FeSi and CoSi

Returning to CoSi we are reminded that, in accordance to the Nernst theorem, temperature derivatives of physical quantities level off at low temperatures and tend to zero at $T \to 0$. As seen in Fig. 1- 3, it seems to occur at about $T/\Theta_D \approx 1/6$, where Θ_D-Debye temperature. But this is not always the case as indicated by the temperature dependence of the CoSi elastic constants featured in Fig. 5. One can see that with decreasing temperature the elastic constants of CoSi pass through maxima between 40 K and 70 K and continue to change down to 2.5 K. This may be tied to the Curie-Weiss like increase of the magnetic susceptibility of CoSi below $\sim 50K$ (see Fig. 5), associated with local moment formation.

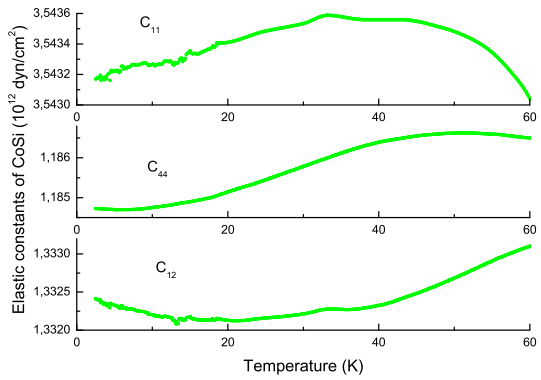

Figure 5. (Color online) Elastic constants c_{11}, c_{12} and c_{44} of CoSi (enlarged view)

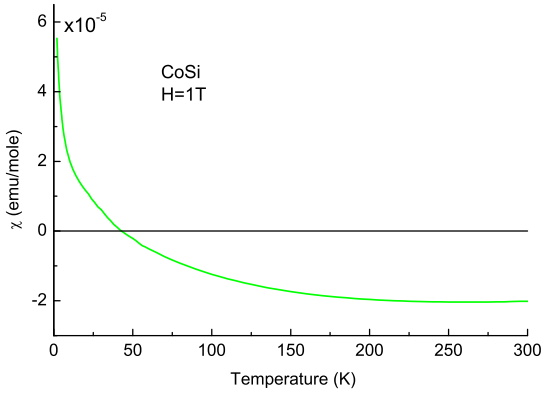

Figure 6. (Color online) Magnetic susceptibility of CoSi

The origin of these moments is probably connected with conduction electron localization at lattice defects that in turn renormalize the phonon spectra of CoSi. Clearly, this is not a complete explanation considering that FeSi, which also features a Curie-Weiss tail, does not display any irregularities in the elastic constants. Along with this unexplained behavior the description of the elastic properties of CoSi cannot be done based on a single a single energy scale like the Debye temperature. Rather an entire spectrum of characteristic energies down to

Table 1. Elastic constants of MnSi, FeSi and CoSi (a-lattice parameters, Θ_D-Debye temperature, calculated from elastic constants)

MnSi a=4.5598Å Θ_D=660 K			
C_{ij}	T=6.5	T=78	T=115
C_{11}	3.2057	3.2045	3.2047
C_{44}	1.2615	1.2582	1.2540
C_{12}	0.8523	0.8574	0.8477
FeSi a=4.483Å Θ_D=680 K			
C_{ij}	T=6.5	T=77.8	T=292.8
C_{11}	3.4626	3.4454	3.1670
C_{44}	1.3916	1.3858	1.2521
C_{12}	1.0576	1.0608	1.1298
CoSi a=4.444Å Θ_D=625 K			
C_{ij}	T=6.5	T=77.8	T=292.8
C_{11}	3.5432	3.5404	3.4529
C_{44}	1.1847	1.1857	1.1593
C_{12}	1.3323	1.3331	1.3128

$\sim$ 1 K may be required.

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