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Physical, thermal and ^{57}Fe Mössbauer studies of $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$

$\text{R}_2\text{Fe}_2\text{Si}_2\text{C}$ (R = rare-earths) compounds crystallise in the monoclinic $\text{Dy}_2\text{Fe}_2\text{Si}_2\text{C}$ -type structure with the C2/m space group. Previous magnetic studies revealed no magnetic phase transition in $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ down to 2 K [1], thus indicating that $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ acts as an ideal non-magnetic reference material for investigating the magnetism of the $\text{R}_2\text{Fe}_2\text{Si}_2\text{C}$ system. Accordingly, we have used $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ as a reference material to estimate the magnetic contribution to the total specific heat of magnetic $\text{R}_2\text{Fe}_2\text{Si}_2\text{C}$ compounds [2-4]. Despite the significance of $\text{R}_2\text{Fe}_2\text{Si}_2\text{C}$ for enhanced understanding of the magnetism of $\text{R}_2\text{Fe}_2\text{Si}_2\text{C}$ compounds, no detailed studies have so far been reported for $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$.

In this work, we report our detailed investigations of the structural and thermal properties, specific heat (C_P) together with ^{57}Fe Mössbauer studies and first-principles calculations on $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$. The thermal expansion of $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ follows the Debye-Grüneisen relation with no pronounced anomalies observed between 20 K and 300 K. By comparison, the C_P data over the temperature range of 2 K - 300 K cannot be described adequately by the Debye model; rather, the C_P data have been described fully by the Debye-Einstein model including anharmonic corrections, suggesting the importance of optical contributions (Einstein terms) to the phonon spectrum in $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$. The low-temperature C_P measurements (2 - 17 K) yield a rather large Sommerfeld coefficient = 16.3(5) mJ/mol. K^2 , reflecting a large density of states (DOS) at the Fermi energy (E_F) which suggests that $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ might be an itinerant ferromagnet. On the other hand, ^{57}Fe Mössbauer spectra measured from 10 K to 300 K show no magnetic splitting, confirming that the Fe atom is in a non-magnetic state. While electronic structure calculations reveal a large DOS at the Fermi energy, the DOS of the Fe-3d states at E_F is only 1.1 states/eV per Fe atom. This value corresponds to $N(E_F)I = 0.51$ which is far below the Stoner criterion for ferromagnetism, thereby establishing that $\text{Y}_2\text{Fe}_2\text{Si}_2\text{C}$ is far from being magnetic.

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