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Physical, thermal and ^{57}Fe Mössbauer studies of $Y_2Fe_2Si_2C$

R2Fe2Si2C (R = rare-earths) compounds crystallise in the monoclinic Dy2Fe2Si2C-type structure with the C2/m space group. Previous magnetic studies revealed no magnetic phase transition in Y2Fe2Si2C down to 2 K [1], thus indicating that Y2Fe2Si2C acts as an ideal non-magnetic reference material for investigating the magnetism of the R2Fe2Si2C system. Accordingly, we have used Y2Fe2Si2C as a reference material to estimate the magnetic contribution to the total specific heat of magnetic R2Fe2Si2C compounds [2-4]. Despite the significance of R2Fe2Si2C for enhanced understanding of the magnetism of R2Fe2Si2C compounds, no detailed studies have so far been reported for $Y_2Fe_2Si_2C$.

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 $Y_2Fe_2Si_2C$. The thermal expansion of $Y_2Fe_2Si_2C$ 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 $Y_2Fe_2Si_2C$. The low-temperature C_P measurements (2 - 17 K) yield a rather large Sommerfeld coefficient γ = 16.3(5) mJ/mol. K^2, reflecting a large density of states (DOS) at the Fermi energy (E_F) which suggests that $Y_2Fe_2Si_2C$ 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 $Y_2Fe_2Si_2C$ is far from being magnetic.

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Primary author(s) : Mr SUSILO, Resta (UNSW Canberra)

Co-author(s) : Mr HSU, Chuang-Han (Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore 117546); Dr LIN, Hsin (Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore 117546); Prof. CADOGAN, Sean (UNSW Canberra); Prof. CAMPBELL, Stewart (UNSW Canberra); Dr HUTCHISON, Wayne (The University of New South Wales)

Presenter(s) : Mr SUSILO, Resta (UNSW Canberra)