Crystal Chemistry of the Superconductor MgB_2

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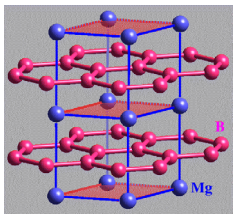
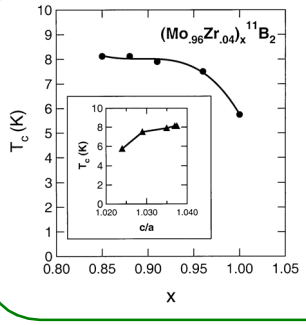
Motivation: Understand how the properties of the superconductor MgB_2 can be changed by inserting vacancy or substitutional defects.

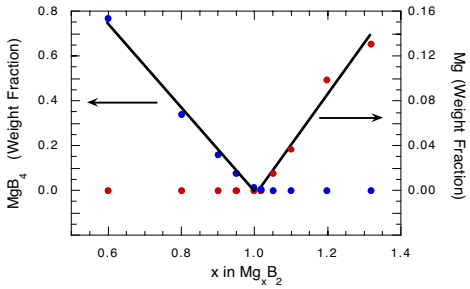


Crystal Structure of MgB_2

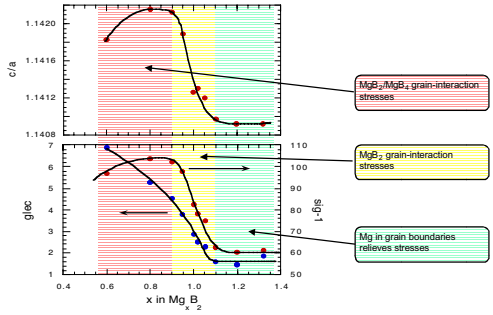
Results:



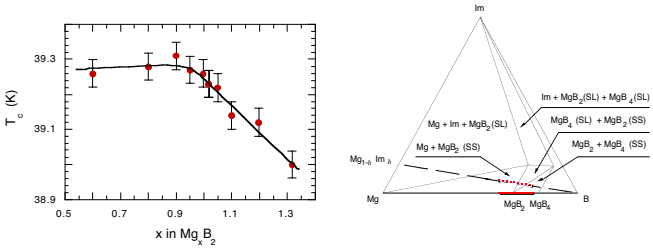
In $(Mo_{0.96}Zr_{0.04})_xB_2$, which has the same crystal structure as MgB_2, T_c can be increased by creating vacancy defects on the metal site.



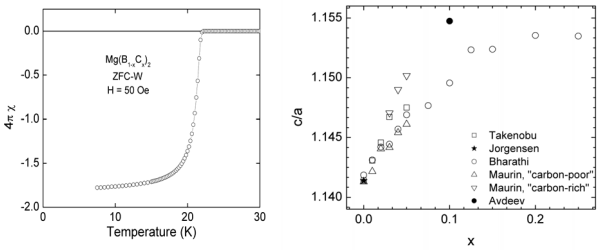
However, when the starting composition of MgB_2 is varied, no vacancies are formed. Instead, MgB_4 or Mg impurities appear. Thus, MgB_2 is a line compound with fixed composition.



Subtle variations in the lattice parameters can be explained in terms of grain-interaction stresses.



A small decrease of T_c with excess Mg can be explained in terms of accidental impurity doping.



Substitution of C on the B site lowers T_c rapidly, but the solubility limit for C is 10%.

Impact: Claims of non stoichiometry are shown to be false. Subtle effects of bulk composition on structure and T_c have other explanations. C is one of the few chemical substitutions that can be made, but the solubility limit is 10%.

Future Work: The observation of effects from accidental impurity doping suggests ways to dope MgB_2 using alloys of Mg.

Structure and Superconductivity in Zr-Stabilized, Nonstoichiometric Molybdenum Diboride, L. E. Muzzy, M. Avdeev, G. Lawes, M. K. Haas. H. W. Zandbergen, A. P. Ramirez, J. D. Jorgensen, and R. J. Cava, Physica C 382, 153-165 (2002); Synthesis and Stoichiometry of MgB_2, D. G. Hinks, J. D. Jorgensen, H. Zheng, S. Short, Physica C 382, 166-176 (2002); Crystal Chemistry of Carbon-Substituted MgB_2, M. Avdeev, J. D. Jorgensen, R. A. Ribeiro, S. L. Bud'ko, P. C. Canfield, Physica C 387, 301-306 (2003)

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