Accepted Manuscript

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PII: S0925-8388(18)32800-7

DOI: 10.1016/j.jallcom.2018.07.299

Reference: JALCOM 47015

To appear in: *Journal of Alloys and Compounds*

Received Date: 17 March 2018

Revised Date: 22 July 2018

Accepted Date: 25 July 2018

Please cite this article as: W.-W. Xu, F. Xia, L. Chen, M. Wu, T. Gang, Y. Huang, High-temperature mechanical and thermodynamic properties of silicon carbide polytypes, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.07.299.

High-temperature mechanical and thermodynamic properties of silicon carbide polytypes

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Abstract

Silicon carbide is widely used as ultra high-temperature ceramics, semiconductors, and pressure sensors with promising potentials for high-temperature, high-endurance, and radiation hardened applications. Daunting difficulties in experimental investigations of thermophysical properties hinder the better understanding of high-temperature material behaviors of silicon carbide. We present a comprehensive study of temperature-dependent mechanical and thermodynamic properties of SiC polytypes by first-principles methods. The obvious anisotropy of linear expansion and elasticity is found for 3C-SiC, while it is not distinct for other non-cubic SiC polytypes. Results show that the temperature dependences of mechanical properties exhibit the softening behavior, in which small linear reduction (~4.4%) in Vickers hardness and shear modulus but large linear reduction (~7.0%) in Young's modulus are detected. The heat-resistant properties of SiC polytypes are ranked as 3C-SiC < 4H-SiC < 6H-SiC <