ATOMIC DIFFUSION MECHANISMS IN TITANIUM CARBIDE

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Transition-metal carbides and nitrides combine ceramic-like properties (high melting point, hardness, and corrosion resistance) with metal-like properties (high electrical and thermal conductivity). These compounds are therefore highly suitable for many existing and emerging high-temperature applications [1]. Understanding atomic defects and diffusion in refractory compounds is important for controlling their properties during manufacturing and service [2]. While monovacancies can fully account for the self-diffusion in Group-IV metal nitrides [3], understanding the diffusion mechanisms of metal atoms in the corresponding carbides represents a challenge due to the extremely high formation energy of a metal vacancy [4,5]. An overview of recent *ab initio* studies of point defects, defect clusters, and diffusion mechanisms in titanium carbide will be given [4–7]. The focus will be made on the Ti self-diffusion mechanisms in TiC mediated by various defect complexes involving vacancies, self-interstitials, and/or oxygen impurity atoms.

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1. Toth L. E. (ed.) Transition Metal Carbides and Nitrides. Academic Press, New York, 1971.
2. Andrievskii R. A. // Powder Metallurgy and Metal Ceramics. 2011. V. 50. Nos.1-2. P. 2; [Russian original: Poroshkovaya Metallurgiya (Kiev). V.50, Nos.1-2. P. 5].
3. Gambino D., Sangiovanni D. G., Alling B., Abrikosov I. A. // Phys. Rev. B. 2017. V. 96. Art. No. 104306.
4. Razumovskiy V. I., Ruban A. V., Odqvist J., Korzhavyi P. A. // Phys. Rev. B. 2013. V. 87. Art. No. 054203.
5. Razumovskiy V. I., Popov M. N., Ding H., Odqvist J. // Comput. Mater. Sci. 2015. V. 104. P. 147.
6. Sun W., Ehteshami H., Korzhavyi P. A. // Phys. Rev. B. 2015. V. 91. Art. No. 134111.
7. Sun W., Ehteshami H., Kent P. R. C., Korzhavyi P. A., to be published.