

Molecular-dynamic analysis of liquid niobium structure with iron and hydrogen atoms impurities

© Eduard A. Pastukhov, Andrey A. Vostryakov,* Nicolay I. Sidorov,⁺ and Victor P. Chentsov

Laboratory of Metallurgical Melts Physical Chemistry. Institute of Metallurgy, UrD RAS.

Amundsen St., 101. Yekaterinburg, 620016. Russia. Phone: +7 (343) 267-88-93. E-mail: nik@imet.mplik.ru

*Supervising author, ⁺Corresponding author

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Abstract

Hydrogen and Iron diffusion factors in the Niobium melts are estimated by means of molecular dynamic model. Obtained results are compared to literary data on impurities removal from Niobium in the plasma-arc melting at Hydrogen presence, as well as in vacuum-arc melting. Electric field effect to Iron removal process is estimated.