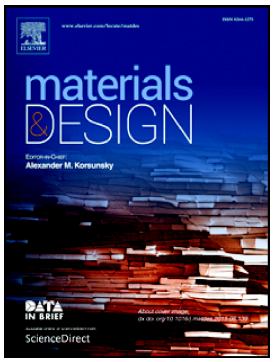
Accepted Manuscript



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PII: S0264-1275(17)30932-2
DOI: doi:10.1016/j.matdes.2017.10.012
Reference: JMADE 3410

To appear in: *Materials & Design*

Received date: 12 April 2017
Revised date: 4 October 2017
Accepted date: 6 October 2017

Please cite this article as: O.M. Krasilnikov, A.V. Lugovskoy, Yu.Kh. Vekilov, Yu.E. Lozovik , Nonlinear elastic properties of the polycrystalline refractory metals at Megabar pressures: Theoretical approach. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jmade(2017), doi:10.1016/j.matdes.2017.10.012

Nonlinear Elastic Properties of The Polycrystalline Refractory Metals at Megabar Pressures: Theoretical Approach

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Abstract

We present the theoretical technique for the calculation of nonlinear elastic properties of polycrystals in the presence of hydrostatic pressure. For the isotropic aggregates of single-crystal grains with cubic or hexagonal structures at given pressure we define the Lamé constants and express them through the second and third order single-crystal elastic constants. We present the calculated third order Lamé elastic modules of polycrystalline W, Mo and Ru in the pressure range of 0 – 600 *GPa*. The results agree with available experimental data. The obtained values can be used for the prediction of properties for these materials at high pressures and finite deformations. We show, that the methodology can be effectively used with *ab initio* calculations techniques to obtain the data on elastic properties of practical importance.

Keywords: properties modeling; nonlinear elasticity; high pressure; metals; ab initio; Lamé constants

1. Introduction

The elastic constants characterize the mechanical response to external loading. The second order elastic constants (SOECs) define a linear response and the higher order elastic constants (third, fourth etc.) characterize the nonlinear response of materials to finite deformations [1]. The third order elastic constants (TOECs) which reflect the anharmonic

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