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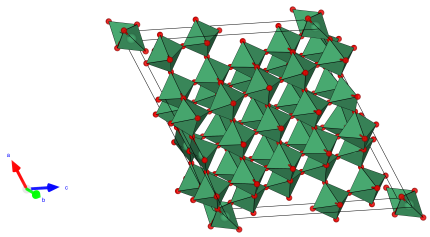
Fitting of New Classical Interatomic Potential for Nb_2O_5 in Phase H by means of advanced algorithms and First Principles calculations

Gómez Fabián[1*], Loyola Claudia[1†], and Valencia-Balvín Camilo[2]
[1]Facultad de Ciencias Exactas, Departamento de Física, Universidad Andrés Bello, Sazié 2212, Piso 7, Santiago, Chile.
[2]Institulo Tecnológico Metropolitano ITM, calle 73 N° 76A-354 Vía al Volador, Medellín, Colombia.
∗fabian.gomez.ingfis@gmail.com, †claudia.loyola@unab.cl

Introduction

We present a novel inter-atomic potential for H phase of Niobium Pentoxide, H-Nb_2O_5, Figure 1. A polymorphic semiconductor with a wide band gap widely used on different technological applications [1]. Here, by using first-principles calculations of structures and energies, we determine a set of numerical parameters related to a specific functional form of inter-atomic potential [2]. By defining an inter-atomic potential for Nb_2O_5, we can study complex, large-scale structures, which are out of the scope of standard first-principles simulations.

Figure 1: *H-Nb_2O_5 phase structure of 29 Nb and 70 O atoms. The structure is monoclinic with lattice vectors $a = 21.153$ Å, $b = 3.8233$ Å, $c = 19.356$ Å and angle $\beta = 119.8°$.*



The fitting technique combines the Genetic Algorithm and Particle Swarm Optimization to minimize the objective function related to the structure and data provided by *Ab Initio* calculations, using the MPI interface to support multiprocessing in search of every parameter aforementioned. Our results show a good agreement of the structural properties of Nb_2O_5 in the H-phase. Despite the large set of different stages present in Nb_2O_5, our results give clear insights into the scope of the inter-atomic potential and possible generalization for other cases. Our work is a step forward in understanding Niobium Pentoxide's phases and their application under different conditions.

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