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Temperature induced disorder in β-Zr

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The behavior of free surfaces and of grain boundaries of a *bcc* Zr system, close to the melting temperature, are investigated using molecular dynamics in combination with a tight-binding potential. Our system consists in more than 5000 atoms and the potential incorporates both two- and many-body terms. The evolution of the disordering sequence, as the temperature increases, is studied quantitatively and illustrated graphically. We find that a progressive disordering process takes place, both at the free surfaces and at the grain boundary, as the melting point is approached. For these two cases the process turns out to be quite similar.

Keywords: Surface melting; molecular dynamics; grain boundary; Zirconium

Se estudia, por medio de simulaciones de dinámica molecular, el comportamiento respecto de la temperatura tanto de las superficies libres como de un borde de grano en Circonio con estructura cúbica centrada en el cuerpo. El sistema consiste en más de 5000 átomos y el potencial usado es del tipo *tight-binding*, que incorpora términos de dos y de muchos cuerpos. Se describe la evolución del sistema de acuerdo al aumento de la temperatura, encontrándose que se desarrolla un desorden progresivo tanto en las superficies libres como en el borde de grano a medida que se alcanza el punto de fusion. En ambos casos este proceso resulta ser similar.

Descriptores: Fusión superficial; dinámica molecular; borde de grano; Circonio

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1. Introduction

The theoretical understanding of the melting process in the vicinity of metallic surfaces and interfaces has recently attracted a great deal of interest, motivated in part by the abundant experimental information now available [1]. In fact, new laboratory techniques allow to extract detailed information, at the atomic level, on phenomena that take place close to the melting point and which still are not completely understood.

In this contribution we study, using molecular dynamics (MD), the temperature induced disorder in the neighborhood of free surfaces as well as grain boundaries of β-Zirconium. Zr is the main ingredient of both zircalloy and the Zr-Nb alloy, which are extensively used in the nuclear and chemical industries due to their topnotch mechanical and corrosion resistant properties. Pure Zr exhibits, under atmospheric pressure, a structural phase transition at a temperature of $T = 1136$ K, from the low T hexagonal close packed *hcp* α-Zr phase to the β-Zr, high T, body centered cubic *bcc* phase. In single crystal structure Zr melts at $T_m = 2125$ K. For technical application purposes Zr is used in policrystalline (zircalloy) and in coexisting α- and β-Zr phase forms [2]. It thus seems natural to investigate this material at a microscopic level, in particular, what occurs in the vicinity of surfaces, interfaces and grain boundaries

This paper is organized as follows: after this introduction we present the model, the potential used, and an outline of the procedure to implement the computations, in Sect. 2. The results thus obtained are given in Sect. 3 and the paper is closed, with a discussion and the drawing of conclusions, in Sect. 4.

2. Model, potential and computation procedure.

Our system consists in more than 5000 atoms and the MD simulation is carried out in the microcanonical *ensemble*. The potential we employ is a *tight-binding* [3] one, and incorporates both a two-body and also a many-body term, which allows to obtain satisfactory quantitative agreement with experiment.

We start establishing the most stable zero temperature configuration by means of static molecular techniques. Thereafter the MD simulation itself is undertaken. The order-disorder transition which the system undergoes is studied qualitatively by means of graphic representations of the particle positions, and quantitatively through the static structure factor.

The MD simulations were carried out for a rectangular section bar made of 5004 Zr atoms arranged forming a *bcc* structure, which includes a tilt grain boundary (GB) near the center of the bar, as illustrated in Fig. 1. As is well known [4] in an actual crystal several types of GB's do coexist. Most measurements yield an average of the effects that all the GB's which are present originate. In our calculations we have chosen a 36.9° $\Sigma = 5$ (031) GB, which is conveniently simple and has been widely used in the literature [5].