รูปแบบ Abstract (บทคัดย่อ)

Project Code: MRG6080253

(รหัสโครงการ)

Project Title: "Universal Characteristics of Grain Boundary Energy Distributions in Body-Centered Cubic Metals"

(ชื่อโครงการ) "ลักษณะร่วมของการกระจายตัวของพลังงานของขอบเกรนในโลหะที่มีโครงสร้าง ผลึกแบบบอดี้เซนเตอร์คิวบิค"

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Body-centered cubic (BCC) polycrystalline metals are widely used in many industrial applications such as metal components for automotive parts, refractory metals for spacecraft, and structural materials for nuclear power plants. The reliability and performance of the polycrystallines are strongly influenced by the relative grain boundary population distribution, known as a grain boundary character distribution (GBCD). Because the GBCDs are primarily influenced by grain boundary energy distributions (GBEDs), these GBEDs are certainly necessary for materials design and processing. Because it is not possible to measure or simulate GBEDs for every BCC metal, it is necessary to have a simplifying principle that generalizes grain boundary energies for every BCC metal. Recently, the principal investigator (PI) reported that the simulated grain boundary energies in BCC metals (Fe and Mo) were strongly correlated [1]. Because of the limited data set, the correlation might not be generalized to the other BCC metals. The objective of this proposal is therefore to investigate the characteristics of grain boundary energy distributions in BCC metals (Fe, Mo, Nb, and W) by using atomistic computer simulations. It is expected that the grain boundary energy function for the BCC metals derived in the present study would be greatly benefit to the "materials by design" research and also promote the development of smart manufacturing for automotive parts industries in Thailand.

Keywords : Grain boundary energy, Body-centered cubic metals, and Atomistic computer simulation