



## The Role of Computation in Metallic Alloy Developments

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By Adewumi Popoola

LAP Lambert Academic Publishing Jan 2015, 2015. Taschenbuch. Book Condition: Neu. 220x150x7 mm. Neuware - The formulation of quantum and statistical mechanics in the 20th century has provided the needed motivation for quantitative and predictive theories of metallic alloys. The various theories are encouraged by believes that they will lead to the formulation of better performing, more sustainable, and cost effective materials. Most data on the physical, thermodynamics and the mechanical properties of alloy systems are lacking and computation is believed to be a good starting point in experimental alloy developments. It can fill obvious data gaps and give insights into factors that govern materials phase formation and stability. This book is intended for material scientists and experimenters who are skeptical of utilizing computation to guide their experiments. The book begins with an introduction on metallic alloys in chapter 1. The ab initio Density Functional Theory and the Molecular Dynamics computation approaches are discussed in chapters 2 & 3. Methods for obtaining data on the physical properties of metallic alloys are discussed in chapters 4 & 5. Many calculated results and experimental data are discussed in chapter 6 and an outlook/conclusion given in chapter 7. 120 pp. Englisch.



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