Amorphous Materials: Modeling of Structure and Properties : Proceedings of Symposium; V. Vitek; 347 pages; 1983; Metallurgical Society of AIME, 1983; 9780895204592

Simulations of the structure and properties of amorphous silica surfaces. Jeanette M. Stallons, Enrique Iglesia. â^—.Â The structure and transport properties of solid surfaces have been described using models of varying complexity and rigor without systematic comparisons among available methods. Here, we describe the surface of amorphous silica using four techniques: (1) an ordered surface created by cutting the structure of a known silica polymorph (-cristobalite); (2) an unrelaxed amorphous surface obtained by cutting bulk amorphous silica structures created by molecular dynamics methods; (3) a relaxed amorphous surface created by relaxing the amorphous surface; and (4) a random surface created by. models of atomic arrangements in amorphous materials. The earliest ideas of Bernal on. the structure of liquids were followed by experiments and computer models for the packing. of spheres. Modern approach is to carry out computer simulations with prediction that can.Â and properties of amorphous thin ï¬lms has been described by Fuxi Gan [52]. Thin layers between crystalline grains may also exist in amorphous state, as described by Gleiter [53]. In fact, the original concept in physical metallurgy of â€œamorphous cementâ€ at the grain boundaries was. proposed nearly a century ago by Rosenhein, as recounted in the book by Cahn [54]. 3. Density Fluctuations, Transport of Atoms, and Solidiï¬cation. Structures and properties of amorphous silicon carbonitride (a-SiCN) materials are studied using density functional methods. Topologicaly different models of a-SiCN with 112-156 atoms each were generated from continuous alternating random networks. The networks have distinct topologies which result in a different chemical bonding in the investigated structural models. A first model consists of Si-N and Si-C bonds only. For such materials with â€œanionicâ€ carbon we found the highest bulk modulus. However, the network strain is largely due to the high SiC content, resulting in bond ruputre and red and Amorphous Cluster 132 Summary of a-Ar IAS Structure 132 IAS Model of a-NiNb Alloy 133 Introduction 133. VII. VIII.Â Preface This book is intended primarily for students of materials science and related ï¬elds who want to acquire a fundamental understanding of the atomic arrangements in amorphous solids. A concomitant aim of the book is to provide an appropriate and consistent methodology and vocabulary for describing the atomic structure of amorphous solids. The book may also be of interest to theoreticians, for this is a relatively new ï¬eld of science, open to further evolution and requiring formal proofs of some of the concepts contained herein.Â I am grateful to Professors Fundamentals of Amorphous Solids: Structure and Properties, First Edition. Zbigniew H. Stachurski. Ovshinsky, S.R., â€œFundamentals of Amorphous Materials,â€ in Physical Properties of Amorphous Materials, Institute for Amorphous Studies Series, vol. 1, D. Adler, B.B. Schwartz, and M.C. Steele, eds., Plenum Press, New York, (1985) 105â€“155.Google Scholar. 5. Ovshinsky, S.R. and Sapru, K., â€œThree Dimensional Model of Structure and Electronic Properties of Chalcogenide Glasses,â€ in Proc. of the Fifth Int. Conf. on Amorphous and Liquid Semiconductors, Garmisch-Partenkirchen, Germany, (1974) 447â€“452.Google Scholar. 6. Ovshinsky, S.R. and Adler, D., â€œLocal Structure, Bonding, and Electronic Propertie...