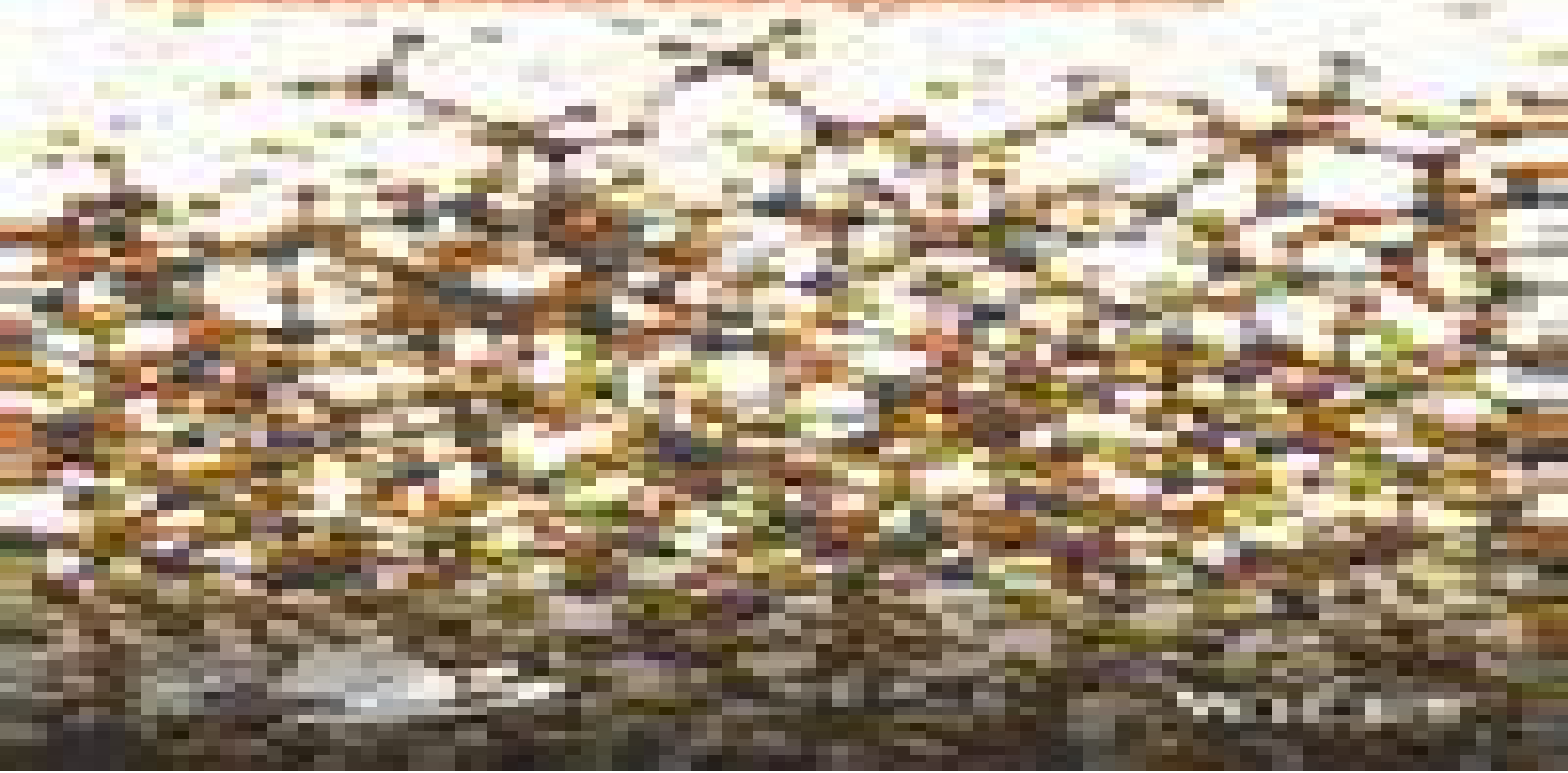


Andrew Chapman, Robert Anderson, and Giovanni

Atomistic Simulations of Glasses

Engineering Science and Technology



Online Atomistic Computer Simulations Inorganic Glasses

Seung Ho Hahn



Online Atomistic Computer Simulations Inorganic Glasses:

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Atomistic Simulations of Glasses Jincheng Du, Alastair N. Cormack, 2022-03-29 A complete reference to computer simulations of inorganic glass materials In Atomistic Simulations of Glasses Fundamentals and Applications a team of distinguished researchers and active practitioners delivers a comprehensive review of the fundamentals and practical applications of atomistic simulations of inorganic glasses The book offers concise discussions of classical first principles Monte Carlo and other simulation methods together with structural analysis techniques and property calculation methods for the models of glass generated from these atomistic simulations before moving on to practical examples of the application of atomistic simulations in the research of several glass systems The authors describe simulations of silica silicate aluminosilicate borosilicate phosphate halide and oxyhalide glasses with up to date information and explore the challenges faced by researchers when dealing with these systems Both classical and ab initio methods are examined and comparison with experimental structural and property data provided Simulations of glass surfaces and surface water reactions are also covered Atomistic Simulations of Glasses includes multiple case studies and addresses a variety of applications of simulation from elucidating the structure and properties of glasses for optical electronic architecture applications to high technology fields such as flat panel displays nuclear waste disposal and biomedicine The book also includes A thorough introduction to the fundamentals of atomistic simulations including classical ab initio Reverse Monte Carlo simulation and topological constraint theory methods Important ingredients for simulations such as interatomic potential development structural analysis methods and property calculations are covered Comprehensive explorations of the

applications of atomistic simulations in glass research including the history of atomistic simulations of glasses Practical discussions of rare earth and transition metal containing glasses as well as halide and oxyhalide glasses In depth examinations of glass surfaces and silicate glass water interactions Perfect for glass ceramic and materials scientists and engineers as well as physical inorganic and computational chemists Atomistic Simulations of Glasses Fundamentals and Applications is also an ideal resource for condensed matter and solid state physicists mechanical and civil engineers and those working with bioactive glasses Graduate students postdocs senior undergraduate students and others who intend to enter the field of simulations of glasses would also find the book highly valuable *Chemical Abstracts*, 1991 Ceramic Abstracts, 1991 **Science Citation Index**, 1995 Vols for 1964 have guides and journal lists Heterogeneities in Metallic Glasses: Atomistic Computer Simulations on the Structure and Mechanical Properties of Copper-zirconium Alloys and Composites Tobias Brink, 2017 Applications of Atomistic Simulation to Radioactive and Hazardous Waste Glass Formulation Development, 1995 Glass formulation development depends on an understanding of the effects of glass composition on its processability and product quality Such compositional effects on properties in turn depend on the microscopic structure of the glass Historically compositional effects on macroscopic properties have been explored empirically e g by measuring viscosity at various glass compositions The relationship of composition to structure has been studied by microstructural experimental methods More recently computer simulation has proved a fruitful complement to these more traditional methods of study By simulating atomic interaction over a period of time using the molecular dynamics method a direct picture of the glass structure and dynamics is obtained which can verify existing concepts as well as permit measurement of quantities inaccessible to experiment Atomistic simulation can be of particular benefit in the development of waste glasses As vitrification is being considered for an increasing variety of waste streams process and product models are needed to formulate compositions for an extremely wide variety of elemental species and composition ranges The demand for process and product models which can predict over such a diverse composition space requires mechanistic understanding of glass behavior atomistic simulation is ideally suited for providing this understanding Moreover while simulation cannot completely eliminate the need for treatability studies it can play a role in minimizing the experimentation on and therefore contact handling of such materials This paper briefly reviews the molecular dynamics method which is the primary atomistic simulation tool for studying glass structure We then summarize the current state of glass simulation emphasizing areas of importance for waste glass process product modeling At SRS glass process and product models have been formulated in terms of glass structural concepts Atomistic-simulations of Silicate Glasses Seung Ho Hahn, 2020 Silicate based glasses are one of the most versatile materials in terms of technological perspective with a wide range of industrial applications In most cases glass products are exposed to various aqueous environments either humid air or liquid water and subject to physical contact with foreign objects which leads to deterioration of chemical and mechanical properties of glass surfaces

Therefore understanding their interactions with adsorbed interfacial water molecules is critical as it can provide physical insights needed for rational design of more durable glasses. Experimental characterization approaches have been applied to tackle difficult problems associated with the complex nature of glass surfaces but they are often limited by the time scale resolution. As a result they have failed to offer important structural characteristics and chemical reaction mechanisms under dynamic processes happening at the glass surface. To complement the challenges that experimental endeavors are encountering this dissertation aims to provide a comprehensive understanding of water interactions of silicate glass surfaces using atomistic scale simulations techniques. In particular ReaxFF reactive force field based molecular dynamics MD simulations are employed to study two distinct surface phenomena i surface water reaction and ii surface mechanochemical wear process. These studies represent the surface damage process of silicate glass in the absence and presence of mechanical actions respectively. The first part of this dissertation describes the water interactions of a silicate glass with readily leachable alkali sodium ions. In this study highly complex surface chemistry including proton water exchange with the sodium ions formation of relatively long living sodium hydroxide ionic complexes at the glass surface and eventual dissolution of those ion pairs into the water phase are described. Also surface mapping of water binding energy to the glass surface is evaluated at different stages of the glass water reaction which would be relevant to assess the chemical durability of the glass materials based on the glass network topology. After the transport behavior and glass water reaction mechanism at the surface has been identified the mechanochemical wear process of sodium silicate glass rubbed with amorphous silica in the absence and presence of interfacial water molecules is covered in the second part of this dissertation. The effect of water molecules on the shear induced chemical reaction at the sliding interface was investigated and the dependence of wear on the number of interfacial water molecules in ReaxFF MD simulations was found to be qualitatively in reasonable agreement with the experimental data. The large scale atomistic simulation approaches with ReaxFF reactive force field presented in this dissertation alleviates the limitations of DFT calculations and experiments providing new and meaningful insights on the chemical dynamics associated within the glass water interface.

Computer Simulation and Atomistic Modelling of

Materials Institute of Physics, Atomic Collisions in Solids Group, 1993

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