Composites Part B: Engineering Volume 143, 15 June 2018, Pages 282–291 Nano-engineering of construction materials using molecular dynamics simulations: Prospects and challenges Author links open overlay panelDenvidLauabDavidHuid https://doi.org/10.1016/j.compositesb.2018.01.014 Get rights and content Abstract In recent years, research articles involving molecular dynamics simulations of construction materials have grown significantly in number.Natural Key challenges in nano-engineering Although MD simulations on construction material systems have been an active research area over the past decade, some challenges still overshadow the progress in the molecular modeling and the computational prediction.To reinforce or rehabilitate these structural components for long-term service, FRP composites have been adopted as ideal candidates due to the advantages of high specific strength and specific stiffness, lightweight, noncorrosive, and Bio-inspired design The multifunctional properties of natural materials are attributed to their subtle structures derived from the nature, and offer cues for special functions and inspirations for manipulating material structures.All of these components react with water to generate hydration Fiber reinforced polymer (FRP) The traditional construction materials, such as the aforementioned concrete and wood structural members, suffer from unwanted deformation and degradation when subjected to external loadings at different environmental conditions during engineering applications.Graphical abstract Image 1 Download : Download high-res image (380KB)Download : Download full-size image Introduction The breakthroughs in nano-engineering over the past few decades enable investigations upon intricate phenomena in material systems at the nanoscale, which contributes to the development of strengthened materials with unique features.In this paper, the applications of molecular dynamics simulations in understanding the fundamental deformation mechanism of various construction materials including concrete and cement, fiber-reinforced polymers and related bonded systems upon nano-engineering approach are presented.The modeling scheme using molecular dynamics (MD) simulations for addressing nanostructures and atomistic interactions inside material systems is essential when applying the nano-engineering approach as it is required to evaluate atomistic movements based on material science and inherent behaviors of actual materials.Traditionally, the classical continuum mechanics theories have been the basis for most computational methods used in various engineering fields including civil and mechanical engineering; examples are finite element analysis, finite difference method, finite volume and boundary element methods.The enrichment of forcefields for various interactions satisfies the need of describing the interactions between dissimilar components as well as between materials and external surroundings such as water or other molecules in solvent environments, which cause the structural change in construction materials and affect material properties in a long run.This review demonstrates the capability of nano-engineering for research of construction materials, which is a breakthrough from the traditional idea which normally sticks to the investigations of construction materials using macroscale models only to an innovative approach which integrates two extreme and disconnected fields (i.e. discrete versus continuum) as a whole.In this paper, the nano-engineering approach using MD simulations on the studies of construction materials, as well as the recent progress on the fundamental understanding of construction materials and their behaviors, is reviewed with an emphasis on the linkage between the nanoscale and the macroscale, and the transition from research to practical

applications.The nano-engineering employs the perspective from the nanoscale towards in-depth understanding of underlying properties and deformation mechanisms that govern macroscopic performance of construction materials, and the procedure is implemented as shown in Fig.Concrete and FRP composites are man-made construction materials, and some inside ingredients are manufactured by artificial synthesis, which can improve the material properties to certain extent while lots of efforts are still required to understand the enhancement mechanism.To improve the calculation efficiency in the iterative processing, different numerical methods have been developed, for example, Verlet integration, leapfrog integration, velocity Verlet integration and predictor-corrector integration [6].Nano-engineering, as a concept about manipulating material structures for creating new materials or modifying existing materials, highly depends on the understanding of materials at the nanoscale, where molecular dynamics simulation becomes an effective and powerful investigation tool.It has been reported that most of construction materials look good when only focusing on their performance in a short term, but they can significantly deform or even fail upon external loadings (which is within its designed capability) in natural environments over a certain period of time due to the deterioration within materials or the interaction between materials and surroundings [[1], [2], [3]].MD simulations serve as effective computational experiments to characterize material properties and predict mechanical responses, which can be used to verify theoretical hypotheses.The compositions of construction materials always refer to different physical and chemical components, and the molecular models for these complicated structures in MD simulations are required to correctly mimic the corresponding material systems.More importantly, the use of nano-engineering in the field of construction materials can help us discover various fundamental failure mechanisms inside material systems and such information provides lots of inspirations for structural design, which is beyond the scope of civil engineering.In MD simulations, materials can be treated as aggregation of atoms which are regarded as classical (non-quantum and subjected to Newton's Laws of motion) mass particles.To resolve the limitation in both the length scale and the time scale, the multiscale modeling for construction materials is proposed that can link MD results to microscopic observations so as to interpret material behaviors.MD simulation represents a powerful tool for potential applications in various research fields including physics, chemistry, biology, bio-engineering and medicine [5,6].Widely used construction materials like concrete, fiber reinforced polymer (FRP) and their related bonded structures are selected as representative material systems here.1.2.