



The molecular dynamics description of Polycaprolactone coating effect on mechanical behavior of Polycaprolactone/BG-AK bio-nanocomposites

Xiuli Du ^a, Dheyaa J. Jasim ^b, S. Mohammad Sajadi ^c, Maboud Hekmatifar ^d, Soheil Salahshour ^{g, h, i}, Roozbeh Sabetvand ^e, Ahmadreza Arefpour ^f, Davood Toghraie ^d

Show more

+ Add to Mendeley Share Cite

<https://doi.org/10.1016/j.ijadhadh.2023.103577>

[Get rights and content](#)

Abstract

In current computational research, the effect of Polycaprolactone (PCL) coating on the mechanical properties (MP) of biomimetic calcium phosphate (BCP)/Baghdadite (BG)-AK nanocomposite (NC) is investigated by using molecular dynamics simulation (MDS). Our study models BCP/BG-AK-PCL samples by Universal Force Field (UFF) and DREIDING potential functions. The outcomes of MDS on the MP of atomic samples are presented by computing physical factors like temperature (Temp), potential energy (PE), Young's modulus (YM), and ultimate strength (US). Physically, MD outputs indicate the physical stability of the BCP/BG-AK-PCL sample after 5 ns. Also, by inserting the PCL coat into the pristine matrix, the YM of this structure reaches 0.39MPa, and the US increases to 20.28MPa. These numerical results show the important effect of PCL coats on the MP of pristine BCP/BG-AK NC, which can be used for clinical applications.