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Optimal design of new structures and nano-materials – computational intelligence approach

Abstract

The lecture consists of three parts.
In the first part short general remarks on criteria of Artificial Intelligence is presented.
The second part will be devoted to application of computational intelligence methods in the form of evolutionary algorithms, artificial immune systems and swarm algorithms to scalar and vector optimization of structures under static and dynamical loads for different criteria. As the particular optimization problem in the form of identification problems using methods of computational intelligence will be presented.
In the third part new potentially 2D nano-materials based on carbon and molybdenum will be generated by the intelligent memetic strategy combining the evolutionary algorithm and the conjugate-gradient optimization technique and molecular model. In this case the main goal of the optimization is to find stable arrangements of carbon atoms under certain imposed conditions. The fitness function is formulated as the total potential energy of an atomic system. The optimized structure is considered as a discrete atomic model and interactions between atoms are modeled using the AIREBO potential. The parallel approach used in computations allows significant reduction of computation time. Validation of the obtained results of new 2D graphene-like materials obtained using the described algorithm are presented, along with their mechanical properties.
Apart from graphene one of the most prominent 2D material is the Single-Layered Molybdenum Disulfide (SLMoS2), which reveals polymorphism at the nano-level. Optimization technique which allows to obtain SLMoS2 heterostructures with desired mechanical properties will be presented.

References

Burczyński T. (et al.), *Intelligent Computing in Optimal Design*, Springer, pp.1-237, **2020.**
Burczyński T. (et al.), *Multiscale Modelling and Optimisation of Materials and Structures*, Wiley, pp. 1-302, **2022.**

Short Bio: Full Professor of Institute of Fundamental Technological Research of the Polish Academy of Sciences, Director of the Institute, Ordinary Member of the Polish Academy of Science (PAS), Ordinary Member of European Academy of Sciences and Art.
His main area of activity is inter- and multidisciplinary scientific research on Information and Computational Science, especially in Computational Intelligence, Computational Mechanics and Computational Materials Science.
He has dealt with an application of intelligent computational systems based on evolutionary algorithms, artificial neural networks, artificial immune systems, swarm algorithms and fuzzy sets in global scalar and vector optimization and identification of structures (T.Burczyński et al, Intelligent Computing in Optimal Design, Springer 2020). He was also the co-author of the original concept an application of artificial immune systems to classification and clusterization of data problems, analysis of multidimensional biological data and coupling artificial immune systems and the game theory. Fuzzy modeling and forecasting financial time series models for the high frequency data using ordered fuzzy numbers is also of his scientific interest.
He has developed a methodology and computer programs for multiscale materials modeling, especially in the field of optimization and identification problems with the use of intelligent systems (T.Burczyński et al., Multiscale Modelling and Optimization of Materials and Structures, Wiley 2022). Recently he has elaborated an intelligent computational methodology for nano-scale optimization of new 2D materials based on carbon and molybdenum.
He has been the principal investigator of several research projects on these subjects.