6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

SHAPE OPTIMIZATION OF MoS_2 BASED MATERIALS

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Key Words: *Molybdenum, Optimization, Bioinspired algorithms, Multiscale.*

The materials with a two-dimensional atomic structure have drawn attention of researchers for years. The carbon based materials are the most analysed one [1]. The one layer materials can be based on many chemical elements like molybdenum or compounds like molybdenum disulphide, tungsten diselenide and others. The stable configurations of atoms in such materials are known but only for typical configurations.
The goal of the paper is to demonstrate method for intelligent design of new flat, atomic, stable nano-structures with prescribed properties based on molybdenum. The paper is focused on shape optimization of one layer material with objective defined as a homogenized material properties. The results of analyses can be used for multiscale modelling of composite with nanostructures.
The optimization is performed with use of bioinspired method combining evolutionary algorithm, particle swarm optimization and artificial immune system. The objective is formulated as a difference between defined mechanical properties (Young moduli) and obtained for vector of design variables. The design variables describes the shape of the void in the flat nanostructure. The new nanostructure with partially removed atoms obtained during optimization process have stiffness as close as possible to the predefined one. The molecular static software is used for stable structure analysis for each set of design variables [2].
The example of results obtained using predefined stiffness in two directions equal to 50N/m and 90 N/m were 53.2N/m and 84N/m.
The presented method allows to design stable nanostructure with predefined material properties.

Acknowledgement
The research is partially funded within National Science Centre Poland project no. 2016/21/B/ST8/02450.

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