MECHANICAL PROPERTIES OPTIMIZATION OF SILICENE BASED NANOSTRUCTURE

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Summary The aim of this work is to present a method for optimizing the mechanical properties of a nanostructure based on Silicene. Optimization is carried out using a parallel evolutionary algorithm and parallel Molecular Dynamics analyses used to determine material properties. Due to high computational costs, optimization was carried out using one of the fastest supercomputers in the world – LUMI installed in CSC in Kajaani, Finland.

OPTIMIZATION PROBLEM FORMULATION

Optimization of the mechanical properties of the shape of 2D nanostructures modified by introducing a void is taken into account in the paper. The nanostructures were modelled on atomic level and optimization process were conducted with use of authors implementations of optimization parallel evolutionary algorithms and LAMMPS[1] software for Molecular Dynamics (MD) analyses. The optimal nanostructures obtained with presented method are building blocks for future gradient materials and nanomechanisms. The optimization problem was formulated as follows:

$$\begin{cases} find & \mathbf{ch} = (g_1, g_2, \dots \dots g_N) \\ minimize & f(\mathbf{ch}) = \left\| \mathbf{P} - \mathbf{P}_{ref} \right\| \\ s.t & g_{iL} \leq g_i \leq g_{iU} \end{cases} \tag{1}$$

where g_{iL} and g_{iU} are lower and upper constraints on design variables values describing shape of the nanostructure. Tensor or vector containing tensors elements **P** denotes the nanostructure mechanical properties obtained for design vector **ch** and $\mathbf{P}_{\mathbf{ref}}$ contains prescribed, reference, mechanical properties of the nanostructure. The minimal difference between current and reference material properties is vector of design variables leading to objective function equal to zero –exact the same reference and obtained properties, but in most cases it is hard to obtain such solution of the optimization problem. The result of optimization with a small difference between the reference and obtained properties is also acceptable. The paper is devoted to optimization of nanostructure taking into account mechanical properties, in our case **P** and $\mathbf{P}_{\mathbf{ref}}$ depend on stiffness of nanostructure with introduced void. The stress – strain relation for small strains can be expressed with Voigh notation as:

$$\sigma_{ij} = P_{ij}\varepsilon_{ij} \tag{2}$$

where ε_{ij} are strain components and P_{ij} contains the elastic constants to be used during objective function evaluation. The shape of nanostructure is modified according to vector of design variables **ch** by introducing elliptic void as shown in Figure 1.

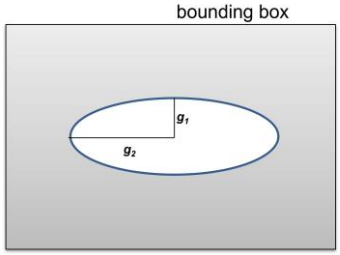

Figure 1. The periodic nanostructure with elliptical void described.

The optimization was performed using parallel evolutionary algorithm [3]. The objective function evaluation for given parameters determining the nanostructure was computed on the base of MD analyses of stretching nanostructure in two directions. The details how to obtain material properties in such approach can be found in [2, 4]. The dominant part taking into account computational costs are MD simulations for each nanostructure. The MD for each design variable can be computed independently and also computations in each direction can be computed separately. This allows to use parallel resources in efficient way.

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OPTIMIZATION RESULTS

The numerical example consists of optimization of Silicene nanostructure with 20 000 atoms and periodic boundary conditions. The ReaxFF potential [5] were used for Si atoms interaction. The heating to 300K and relaxation of the nanostructure with void were performed followed by NPT analysis of stretching with constant strain rate. The elastic constants were computed on the base of stress-strain curve obtained during MD simulations. The evolutionary algorithm consists of 32 chromosomes containing floating point genes. The Gaussian and uniform mutations, simple crossover and tournament selection were used. The optimization was performed on LUMI-C partition of LUMI supercomputer with use of 64 AMD EPYC 7763 processors (4096 processors cores). The results of optimization are shown in Figure 2. The prescribed elastic constants were 75GPa in both directions and for structure presented in Figure 2 for the final solution the constants were 74.99GPa and 75.09 GPa.

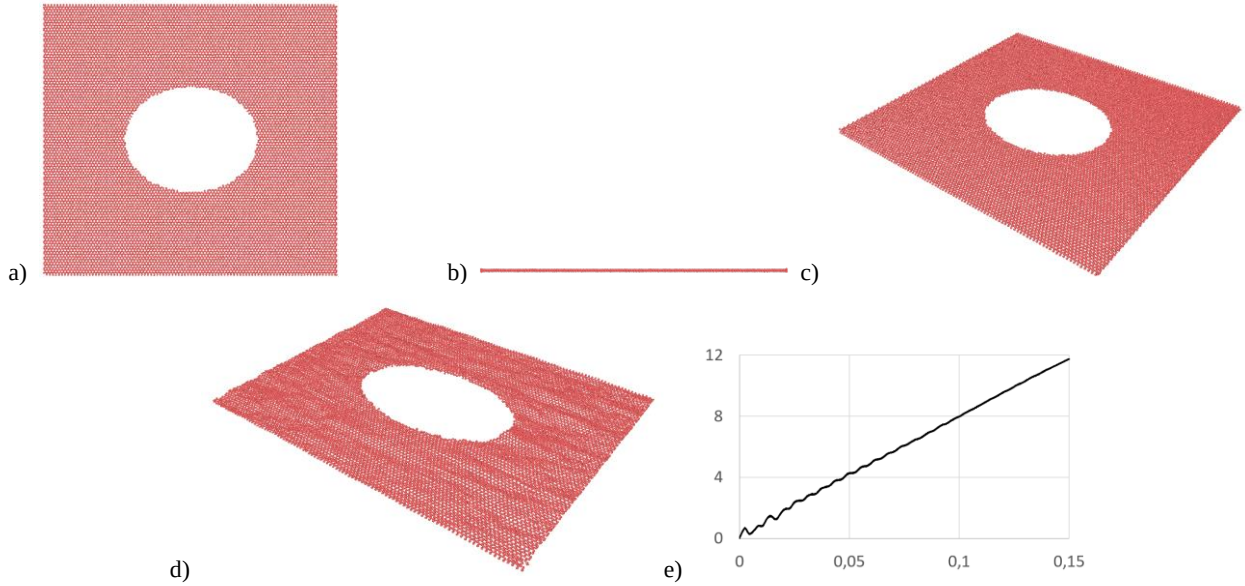

Figure 2. The results of optimization, a) modified Silicene nanostructure view from top, b) view form side, c) isometric view, d) isometric view after stretching in *x* direction, e) stress-strain curve for *x* direction stretching.

CONCLUSIONS

The method of optimization of Silicene based nanostructures with prescribed material properties was presented in the paper. The numerical example presents good agreement of elastic constants of optimized nanostructure with void with prescribed values. The good scalability of parallel evolutionary algorithm and MD allow to obtain results for structure modelled with 20 000 Si atoms and ReaxFF potential.

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