Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Vacancies and Temperature Effects on the Mechanical Properties of Silicene Nanoribbons[1] MA. RAYO CHAVEZ-CASTILLO, Instituto de Fisica BUAP, MARIO ALBERTO RODRIGUEZ-MEZA, Depto. de Fisica, ININ, LILIA MEZA-MONTES, Instituto de Fisica BUAP — The study of two-dimensional materials has been increasing. In the past few years a large variety of these kinds of materials has been studied, such as boron nitride, molybdenum disulfide, and silicene. The main potential application of silicene is found in electronic devices, nevertheless, other possible applications can be found. It is necessary to understand the mechanical properties of the material, because it can help us to determine the stability and useful lifetime thereof. We study vacancies and temperature effects on the Young's Modulus (YM) of silicene nanoribbons (SNRs). To determine their mechanical properties, we perform molecular dynamics simulations at room temperature and at temperatures ranging from 400 to 600 K, and analyze the YM of three square shaped SNRs, whose lengths varies from 3 to 8 nm. Results at room temperature showed that the YM for the ribbons without defects increases with the length in both directions of chirality. On the other hand, for SNRs in the presence of defects (mono-and bivacancies) the YM depends on the defect position. It increases as the vacancy approaches the SNRs boundary. We observed that the higher the temperature, the lower the YM with and without vacancies. However, dependence on the length remains the same.

[1]We acknowledge the financial support from CONACYT Grant. CB/2009/133251 and VIEP-BUAP.

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Date submitted: 14 Nov 2014 Electronic form version 1.4