Bi-layered silicon with strain-induced tunable optical properties for IR applications

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The compatibility with the main-stream silicon technology makes silicene and a few layers of silicon very promising for VLSI beyond 3nm technology node. Similar as its carbon counterpart graphene, energy bandgap (EB) opening presents the most critical demand for potential applications in digital electronics. Based on density function theory, EB opening in bi-layer silicon structures (BLSi) has been obtained under biaxial in-plane strain in our previous works [1, 2]. In this work, we performed a theoretical study of the optical properties of the strained BLSi in mid-IR. It turns out that by applying the in-plane tensile strain, the optical properties of the BLSi can be tuned in a wide range over the entire mid-IR bandwidth.

Our previous works show that buckle-free bilayer silicon structure (Fig.1) can be obtained once the biaxial in-plan tensile strain exceeds 11.2% [1, 2]. As the in-plane strain continuously increases to 16.4%, a direct EB (E_{g_D}) is formed at Γ point in addition to the in-direct EBs (E_{g_ID}) (Fig.2), which promotes direct band transition at IR. To verify it, various optical properties including permittivity, refraction index, and optical conductivity of the BLSi have been calculated versus photonic energy at different strain levels. Figure 3 plots the complex in-plane permittivity of the BLSi under an in-plane strain of 14.8%. The observed absorption (P1 marked in Fig. 3) evidences the direct-band transition. By varying the applied strain, such featured absorptions can be tuned in the range between 0.154-1.056 eV, which covers the entire mid-IR (See supplementary pages). In addition to the featured absorptions, its real part of the permittivity in Mid-IR (<0.2 eV) is of a factor 3 greater than the fully relaxed BLSi, leading to two times enhancement of reflectance. We believe that the buckle-free planar BLSI might open new opportunities of applications at IR.

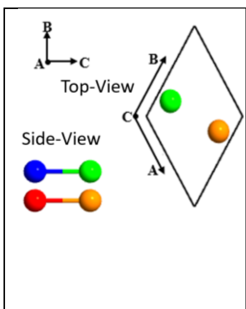

Figure 1. Atomic structure of BLSi

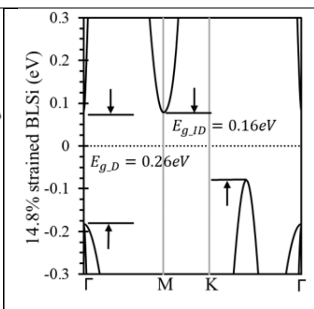

Figure 2. Energy band diagram of strained BLSi

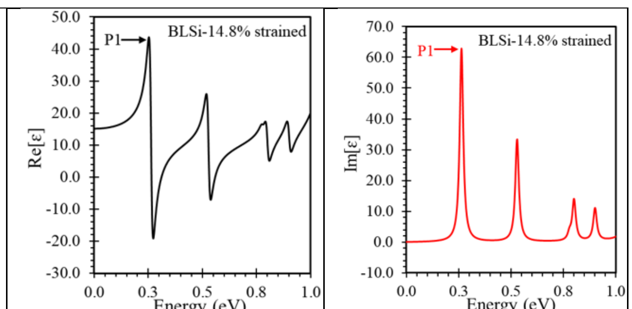

Figure 3. Real (Left) and imaginary (Right) parts of permittivity of BLSi VS photon energy.

[1] Z. Ji, et al, IEEE J. Elec. Mat, 45, 5040 (2016).
[2] K. Vishal, et al, J. Vac. S & T A 41, 022201(2023)

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Supplementary Pages (Optional)

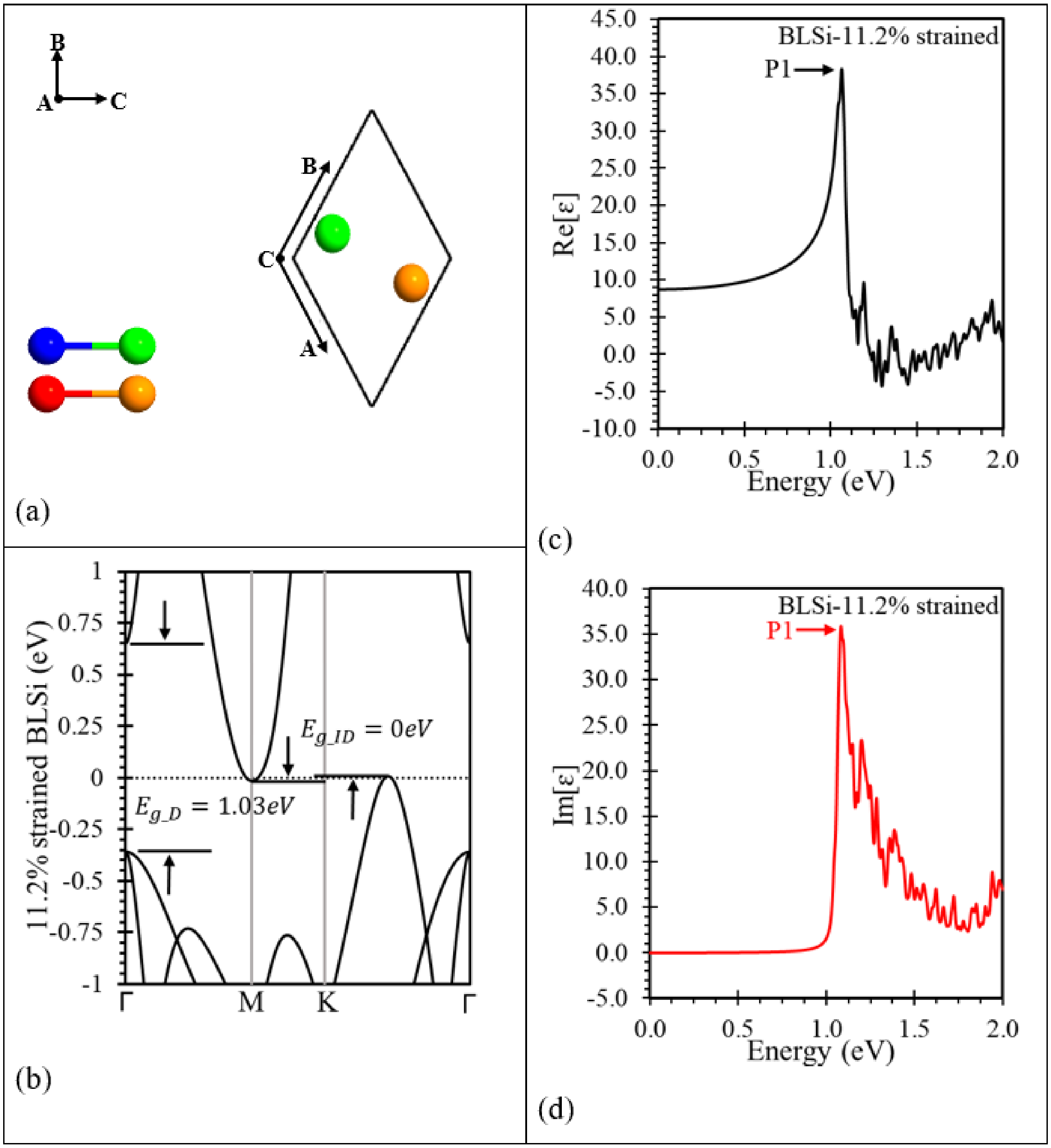

Figure S1. Structural (a), energy band diagram (b), real (c) and imaginary (d) parts of the complex permittivity of a strained BLSi under bi-axial in-plane strain 11.2%. The absorption P1 occurs at 1.056 eV. The buckle height of the strained BLSi is close to zero, resulting in a planar BLSi.

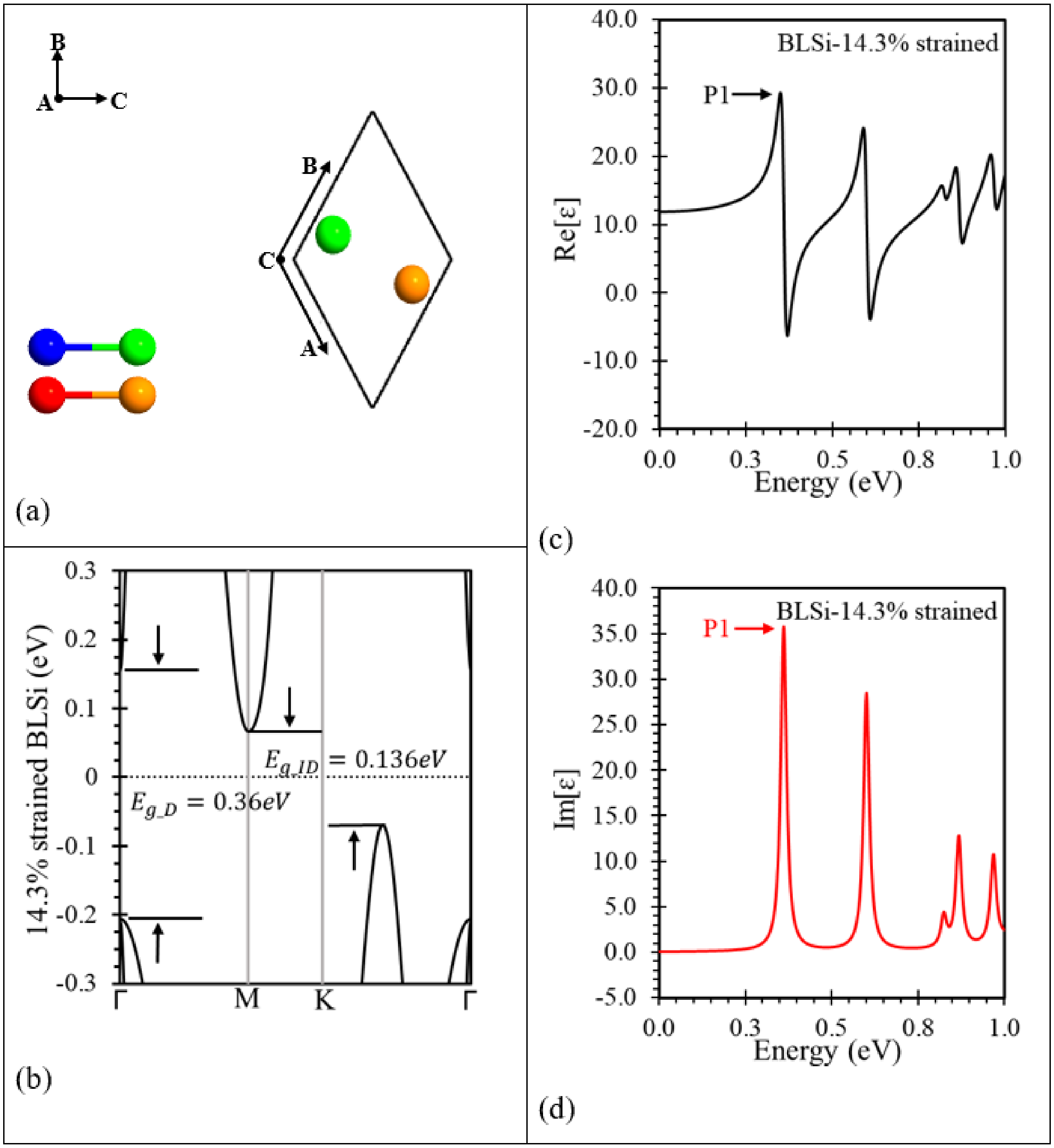

Figure S2. Structural (a), energy band diagram (b), real (c) and imaginary (d) parts of the complex permittivity of a strained BLSi under bi-axial in-plane strain 14.3%. The absorption P1 occurs at ~0.36 eV. The buckle height of the strained BLSi is close to zero, resulting in a planar BLSi.