Supporting Information

Atomic Layer Deposition of Titanium Oxide on Single Layer Graphene: an Atomic Scale Study towards Understanding Nucleation and Growth

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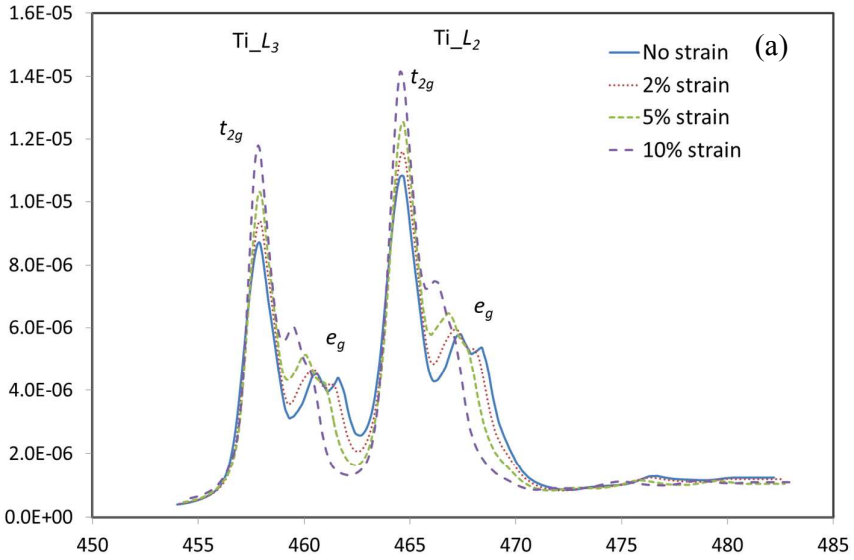
To examine the possibility that the crystalline nuclei are strained TiO_2, EELS simulation of Ti_*L* edge was performed. Calculation of ELNES of TiO_2 was carried out with real space multiple scattering code called FEFF8[1,2]. Self-consistent muffin tin potential and full multiple scattering was obtained using 6.0 Å radius. All calculations were performed using a core hole and an averaged contribution was calculated for Ti_*L* edge EELS spectra. CIF file with lattice parameters *a* and *c* of 4.6518 and 2.9699 Å, respectively was used for the calculations. EELS was also calculated on optimized strained structures where isotropic strain (2%, 5% and 10%) was applied to TiO_2 bulk structure. The results are shown as following:



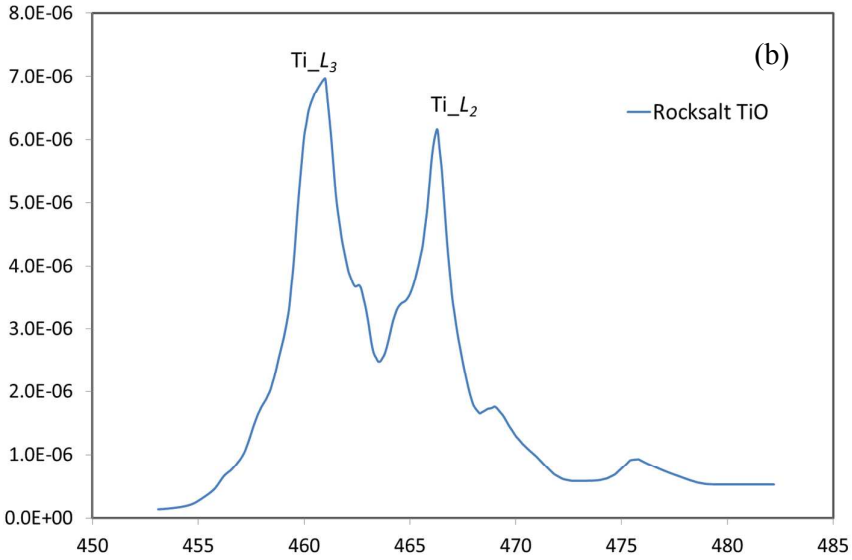


Figure S1: EELS simulation of Ti_*L* edge for (a) anatase TiO_2 under 0%, 2%, 5% and 10% isotropic strain respectively, and (b) rocksalt TiO.

It can be seen that the fine structure of Ti_*L* edge for the strained anatase TiO_2 maintains the same shape with the splitting peaks due to t_{2g} and e_g orbitals. The position of the e_g peak shifts toward a lower energy as the strain increases. For 10% strain, which corresponds to the lattice measurement in Figure 3, both t_{2g} and e_g peaks are still present with a much higher intensity for t_{2g}. This is not consistent with the experimental EELS spectrum for the nucleation sample in Figure 4, which indeed more resembles the simulation from a rocksalt TiO shown in (b). The peaking splitting of the Ti_*L* edge is absent and only the intensity at the energy level of e_g exists. This can be well explained by the molecular orbital (MO) theory as presented in the main text. Therefore, the EELS simulation can rule out possibility that the crystalline nuclei are strained TiO_2 and support the presence of rocksalt TiO at the early stage of nucleation.