Antimonide-based materials, such as gallium phosphide antimonide (GaPSb), that are grown highly mismatched on silicon substrates have interesting applications in high electron mobility III/IV channel layers on Si (001) substrates. As there are no III/IV semiconductors with high electron mobility which can be grown lattice matched on Si, different buffer layers have to be studied and the defect formation within these layers has to be understood in detail to optimize the layer structures for later device application.

To avoid antiphase boundaries penetrating through the Ga(PSb) layer, a gallium phosphide (GaP) layer is grown between the silicon substrate and the Ga(PSb). The antiphase boundaries created by the growth of a polar material on the non-polar silicon substrate annihilate within the GaP [1]. The mismatch between GaP and Ga(PSb) is between zero to twelve percent, depending on the composition. The strain induced by the high mismatch should be relaxed by misfit dislocations at the interface. However, dark-field and high resolution TEM have shown that the bulk contains many other defects like stacking faults, twins and threading dislocations. High resolution TEM and HAADF (high-angle annual dark-field) scanning transmission microscopy investigations of the interface using a double Cs-corrected JEOL 2200FS (S)TEM have revealed that the misfit dislocations mainly are Lomer dislocations and 60° dislocations pairs. Molecular dynamics simulations with Stillinger-Weber potentials have been used to model the structure of the dislocations theoretically. The crystal model has been used as input to simulate the HAADF images with the multislice algorithm and frozen phonon simulation. This contribution shows that HAADF imaging in combination with molecular dynamics simulation is very suitable for defect characterization at the interface of strained materials. TEM is very useful to gain insight on the crystal structure of GaPSb and other metamorphic buffer layers so that their growth can be optimized.

Fig. 1: High resolution HAADF image of the GaP/GaPSb interface with misfit dislocations and stacking faults.