Piezoelectric InAs quantum dots (QDs) were grown on (211)B GaAs surface, by plasma-assisted molecular beam epitaxy (PAMBE). The heterostructure was characterized by high-resolution transmission electron microscopy (HRTEM) methods [Fig. 1(a)]. Combining crystallographic data from plan-view and cross-sectional observations, we came up with the 3D shape model of the QDs depicted in Fig. 1(b). QDs present an asymmetric truncated pyramidal faceted configuration comprising the {100}, {110} and \{21l\} facets, \( l \) varying from 2 to 4. Thus, the pyramid [-111] to [0-11] base-aspect-ratio (BAR) depends on the \( l \) index of the inclined \{21l\} planes, since it influences the out-of-plane angle of the pyramid base tip. Typical BAR values between 1.2 and 1.4 were determined for the InAs QDs. Moreover, the height of the QDs depends both on the \( l \) value and the level of truncation of the apex of the pyramid, which is variable (5-15 nm).

The degree of plastic relaxation of the InAs QDs on GaAs was estimated by Moiré fringe analysis, fast Fourier transform (FFT) of HRTEM images, and geometrical phase analysis (GPA). It was found that the QDs are rather relaxed due to the presence of misfit dislocations (MDs) at the InAs/GaAs interface [Fig 2(a)]. An average value of 6% for the in-plane lattice strain was estimated near the interfacial region. It is noticed, from GPA analysis, that there is an increase of the lattice strain up to 7.1% close to the apex of the QDs, suggesting that in that area there is negligible residual elastic strain [(Fig. 2(b)). The lattice constant increases towards the top of the QDs due to the foil thickness effect and thus, the smaller QDs exhibit the lowest strain. It is clear that strain inside the InAs QDs shows evidence of an anisotropic behavior.

The formation of InAs QDs on (211)B GaAs surface was explored in terms of atomistic reconstructions of the energetically favorable configurations in conjunction with HRTEM results. The pyramidal faceted reconstructions of (211)B GaAs, composed of the \{100\}, \{110\} and \{113\} facets, are considered as the most stable configuration, while another less stable reconstruction is formed by the \{100\}, \{110\} and \{214\} surfaces, which is shown in Fig. 3. However, in addition to the \{214\} surfaces, the \{21l\} surfaces with \( l = 2, 3 \) seem to be experimentally plausible. Since the (211)B surface is faceted, diffusion barriers are much higher with respect to flat surfaces and hence, In adatoms are trapped at the edges of the individual surfaces making the formation of InAs QDs on them favorable with respect to other cleaved flat surfaces (e.g. the \{111\} surface).

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Fig. 1: (a) Plan-view HRTEM image of an InAs QD viewed along the [211] zone axis. Moiré fringes arise due to overlapping of the InAs and GaAs lattices. (b) 3D shape model of the QDs with the l index of the {211} facets being 3.

Fig. 2: (a) Cross-sectional HRTEM image of an InAs QD viewed along the [0-11] zone axis superimposed with the corresponding GPA strain map. (b) Line profiles of the average strain from the areas marked in (a) by dashed lines, along the [211] growth direction.

Fig. 3: Atomistic model of the faceted GaAs (211)B pyramidal surface shape using the method of infinite triangular prism structures.