Valley degeneracy in biaxially strained AlAs quantum wells

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Of the various multi-valley semiconductors, the indirect bandgap semiconductor aluminum arsenide (AlAs) with its bulk three-fold valley degeneracy (Fig. 1) is of particular interest because its heavy anisotropic electron mass allows for large interaction effects, and its near perfect lattice match to the underlying GaAs substrate allows for high-mobility, modulation doped, lattice-matched quantum wells (QWs). Unconventional facets such as (411) have also proven useful in identifying exchange effects like quantum Hall ferromagnetism in AlAs QWs. Evidence for a critical QW width w_c to cross-over from double to single valley occupation has been shown for (001) AlAs wells, as has evidence for single valley occupancy in wide (110) AlAs wells. Dynamic control of the valley degeneracy has been realized with uniaxially strained (001) AlAs QWs to induce valley degeneracy splitting. Such studies can quantify interaction effects, calibrating valley strain susceptibility and valley effective mass.

We derived a complete formalism for calculating electron subband energy and degeneracy in strained multi-valley quantum wells grown along any orientation with explicit results for the AlAs quantum well case [1]. A standardized rotation matrix is defined to transform from the conventional-cubic-cell basis (k_x, k_y, k_z) to the quantum-well-transport basis (k_a, k_b, k_c) whereby effective mass tensors, valley vectors, strain matrices and anisotropic strain ratios are all defined in their respective bases. The specific cases of (001)-, (110)-, and (111)-oriented AlAs quantum wells are examined, as is the unconventional (411) facet, which is of particular importance in AlAs literature. Calculations of electron confinement and strain in the (001), (110), and (411) facets determine the critical well width w_c for crossover from double to single valley degeneracy in each system. The notation is generalized to include miscut angles, and can be adapted to other multi-valley systems.

To estimate the electron subband energy and degeneracy of the different electron valleys one must consider both quantum confinement and strain. By using the next**nano** software [2], we performed calculations for various specific QW orientations in order to determine the critical cross-over width w_c for double to single valley occupation. Our algorithm automatically takes into account for arbitrary growth orientations: (i) strain, (ii) deformation potentials that split and energetically shift the three conduction band edges and thus lift their degeneracy, (iii) rotation of the ellipsoidal effective mass tensors. For each valley the single-band Schrödinger equation is then solved numerically considering different effective masses in the well and barrier materials. Corresponding momentum space illustrations are provided to aid perspective and intuition on visualizing inter-valley scattering (Fig. 2).

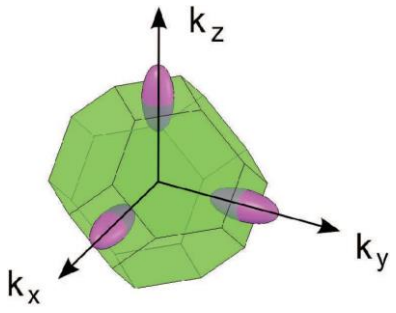

***Fig. 1**: Brillouin zone for bulk AlAs. Crystal symmetry requires three degenerate valleys that are occupied with electrons as indicated by ellipsoidal equi-energy contours.*

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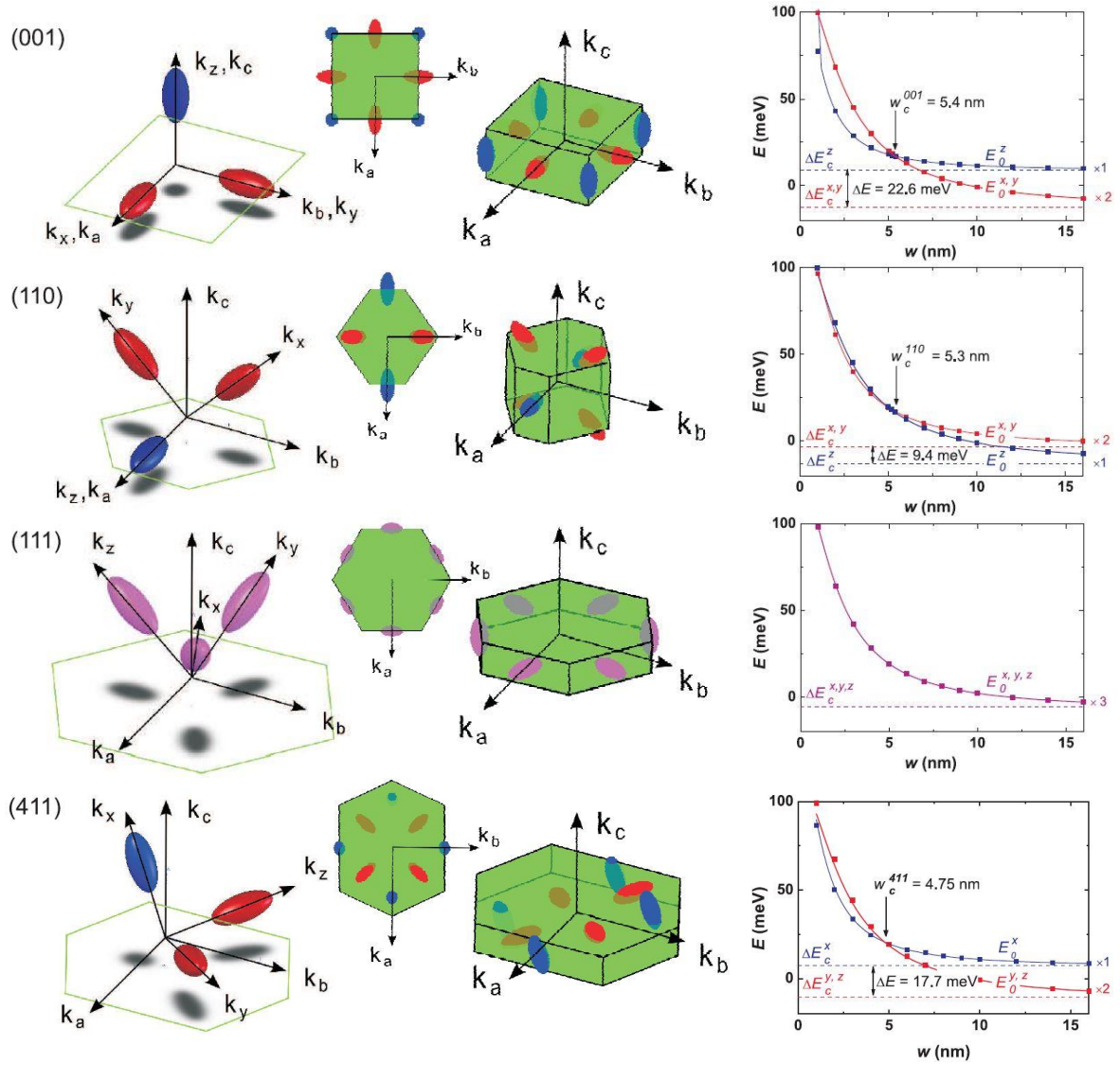

***Fig. 2**: Depiction of the valley degeneracies for various QW orientations. Each row is labeled with its Miller index. Left column: 3D representation of the X-valleys showing both the conventional cubic basis (k_x, k_y, k_z) and the QW transport basis (k_a, k_b, k_c). For (001) and (110) orientations, the doubly degenerate $X_{x,y}$ valleys are red ellipsoids, and the singly degenerate X_z valley is a blue ellipsoid. For the (111)-oriented AlAs QW, the three degenerate $X_{x,y,z}$ valleys are purple, whereas for the (411)-oriented AlAs QW the two degenerate $X_{x,y}$ valleys are red and the singly degenerate X_z valley is blue. Center column: 2D projection and 3D representation of the valley scattering unit cell. Right column: Valley degenerate ground state energy as a function of QW width for a QW barrier of $Al_{0.45}Ga_{0.55}As$ at T = 4 K. Dashed lines represent the calculated strain energy shift of the respective electron valley relative to unstrained AlAs. The results simulated by the heterostructure software next**nano** are depicted with scatter plots.*

[1] S. Prabhu-Gaunkar, S. Dasgupta, S. Birner, C. Knaak, M. Grayson, arXiv: 1009.0336v1 [cond-mat.mes-hall]

[2] www.nextnano.de