Modelling graphene growth by atomistic simulation of 2D polycrystal crystallization - video

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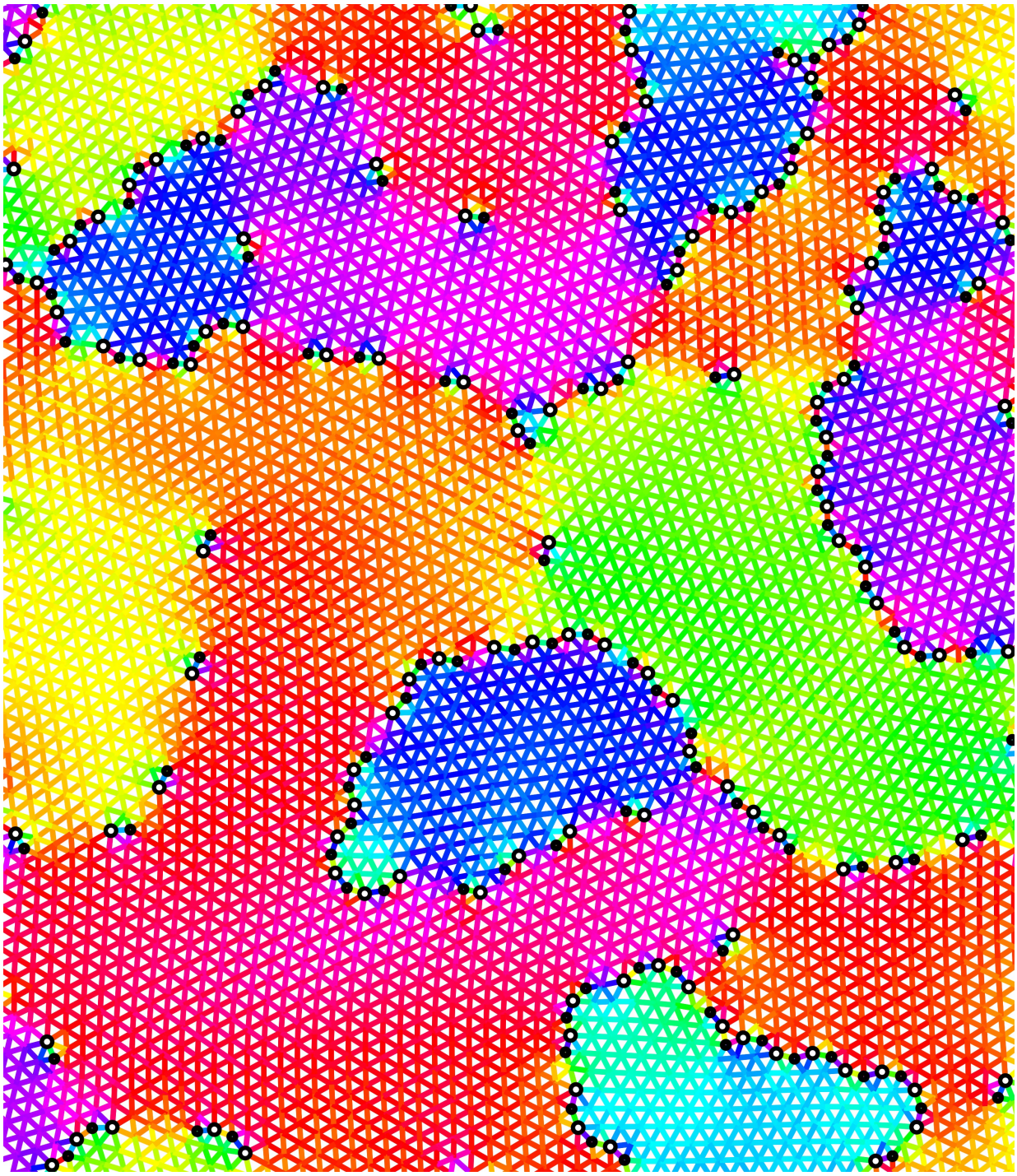
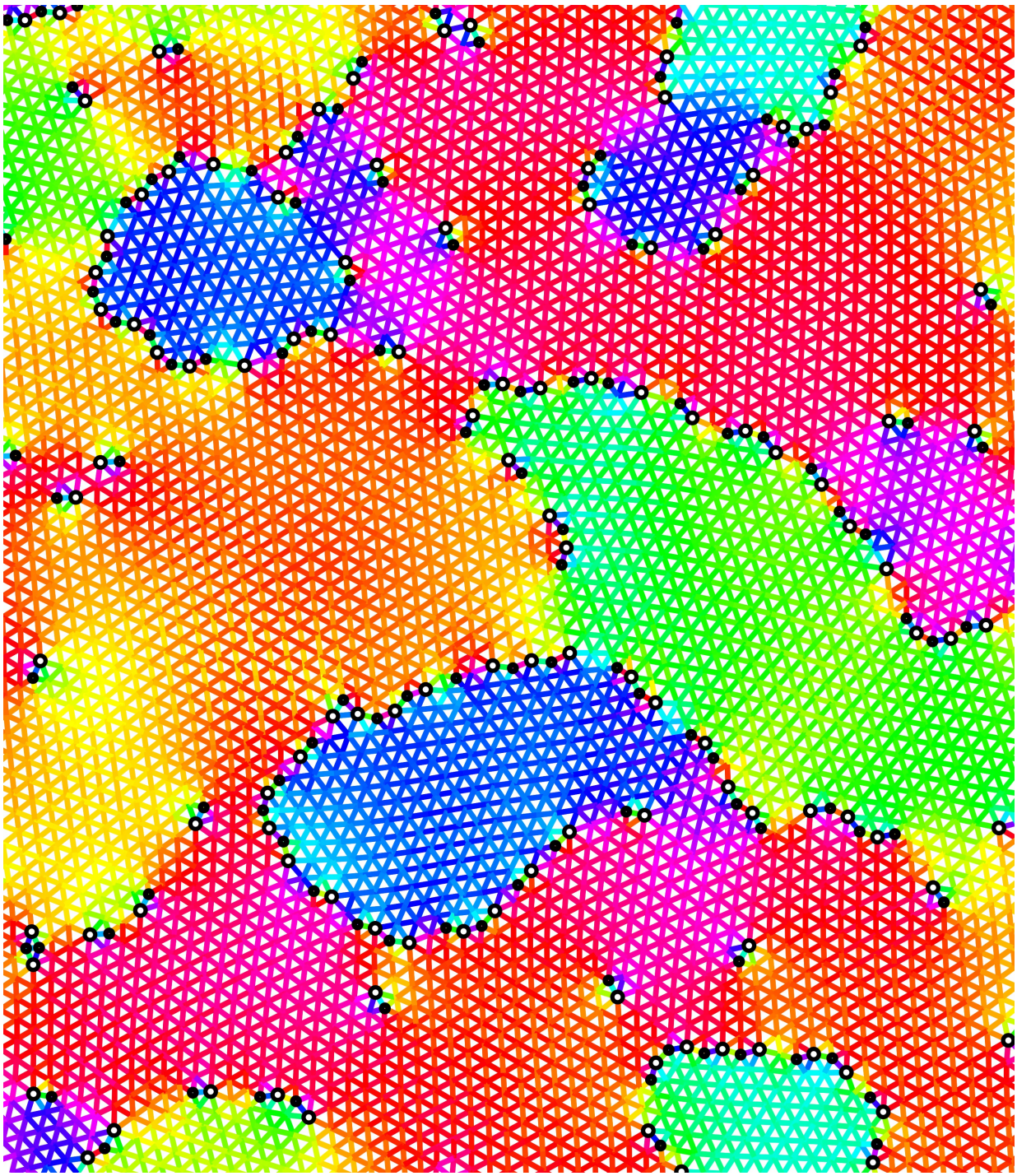
John Werner Cahn first considered close-packed 5-, Hexa-, 7-gons (5H7) in 1965 (5/7 edge dislocations ED) and in lecture “Euler theorem and penta-hepta defects” during MIT 1970 conference “Shaping of tissue by deviation from hexagonal close-packing of cells”, triple junctions (TJ) of grain boundaries (GB) in 2D polycrystal were discussed. In our with Herbert Gleiter paper: “Rearrangement of atoms during GB migration” (Z. Metallkunde 1971) our work with Cahn about coincident GB was announced. Our work with Cahn continued after our lecture “Crystallization as rearrangement of GB and Ed by Voronoi centroidal iterations” at Symp. Phys.Chem. Comp.Films 1978. Modelling extends Boris Yakobson ideas.





Two frames from presented video of atomistic simulaton, mainly Voronoi centroidal iterations from random but uniform initial distributions, dynamically expose ED, 5H7, GB, two opposite (containing additional 5 or 7 disclination) TJ alternating along GB. Also were explored and applied Phase Field Crystals (after Landau, Cahn, Elder), conformal circle-packing, Ricci combinatorial curvature flow ... Crystallization of large 2D bicrystals, with sigma 7 (like Ising kagome phase transition) and sigma 13, 19 ... coincident GB, was presented many times in 2002. 2D polycrystals are emerging as not similar to commonly considered 2D close-packed grains with closed loops of GB, such as seen in 2D crossections of 3D polycrystals and in von Neumann-Mullins grain growth model. Rather more rich configurations of GB, TJ, disclinations, ED, vacancies, interstitials and other 5H7 could be expected in true 2D polycrystals. Cit. from our abstract at Int. Congress of Mathematicians 1983: "Two alternating TJ of GB allows only their even loops." Proof reminds simplest fundamental chirality of oriented clockwise and counter-clockwise triangles. This suggests very fundamental nature and importance of many implications. Two-dimensionality is not a poor "Flatland", but very rich 2D "Glasperlenspiel". 2D is stronger then 3D in structural changes: 5H7 recrystallization, curvatures, topological defects, quasicrystals, phase transitions, percolation ... Life is possible because biomembrane 2D reactions (5H7 changes in lipid rafts, clathrin coated pits ...) surpass surrounding 3D changes. Orientational pinwheels from visual cortex are 2D vortices and anti-vortices, like 5 and 7 disclinations (Gaussian curvature quanta) in 5H7. Very rich, but still poorly understood (graphene promises breakthrough) 5H7 patterns offer enormous power for best coding and control in biology and many other fields with 2D close-packing.