

## Two alternating triple junctions of grain boundaries in graphene and in any 2D polycrystal

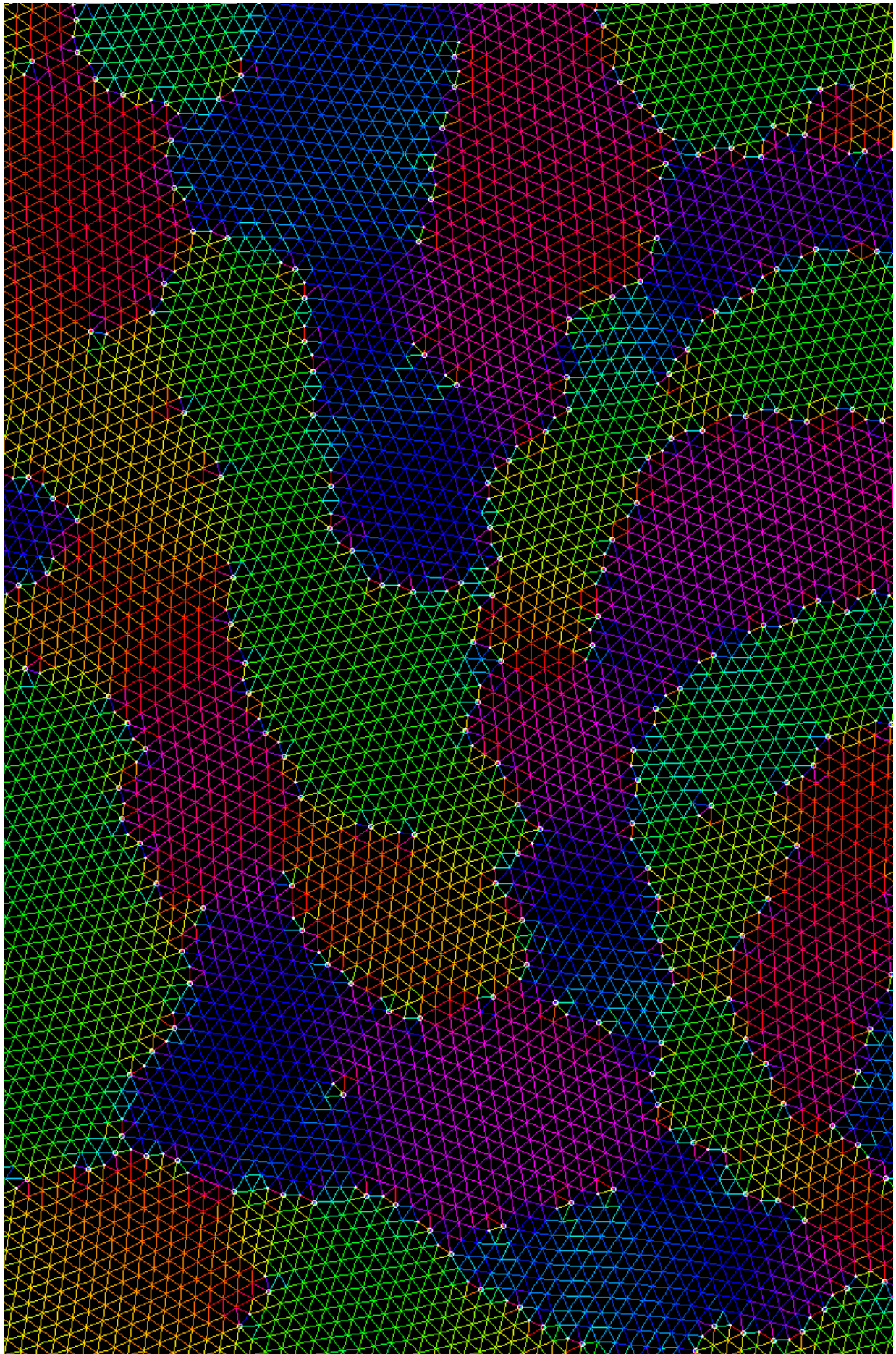
Andrzej Lissowski

Computer Section in Society of the Polish Free University, Slupecka Str. 7/38, Warsaw Poland  
[aliss5h7@engineering.com](mailto:aliss5h7@engineering.com)

Triple junctions (TJ) of grain boundaries (GB) in graphene [1] are recently investigated as main centers for cracks, elucidated by Boris Yakobson [2] as additional heptagonal disclination located in TJ center. Emerging pattern of 5-, Hexa-, 7-gonal close-packing (5H7) in polycrystalline graphene will soon confirm a new understanding of any 2D polycrystal, developed with atomistic simulation. Contrary to repetitively assumed representation of 2D polycrystalline grains pattern with a closed GB loop around each grain, obtained were more rich configurations of GB, TJ with penta- or hepta-gonal disclinations, 5/7 edge dislocations, vacancies, interstitials, 5H7 ... Actually GB rarely form closed loops in simulated atomistic 2D polycrystal, preferably with two possible opposite TJ alternating only around rare even-sided grains. It's proven here that possible are only two opposite kinds of TJ for quilting 5H7 patterns with 2D grains. This old result was rejected till now by many conferences and journals, but now confirmation is ahead. Let misorientation angle  $M$  between neighboring grains  $G1$  and  $G2$  be rotation angle  $A12 < 60^\circ$ , which brings nearest axes  $G1$  to  $G2$  clockwise.  $A12$  and  $A21 = 60^\circ - A12$  could be used for both  $M$  regarded from opposite directions of GB between  $G1$  and  $G2$ . A minimal rotation angle, which brings axes of  $G1$  to  $G2$  counter-clockwise, is equal to  $60^\circ - A12 = A21$ . Following is valid also for such opposite angles, if chosen. Sum of three GB  $M$  angles in TJ is  $< 180^\circ$ , because each GB  $M$  angle is  $< 60^\circ$ . Theorem: Such sum could be only  $60^\circ$  or  $120^\circ$ , because is  $60^\circ \cdot \text{integer}$ . Proof: Angle inside grain, between axes-borders of both  $M$ , is  $60^\circ \cdot \text{integer}$ . Three such angles together with three GB  $M$  angles sum up to  $60^\circ \cdot 6 = 360^\circ$  around flat TJ. Let  $G1/G2$  be fully embedded into a big grain  $G3$ , like inside letter H with horizontal line as GB of  $G1/G2$  and added parallel horizontal parts of  $G1/G3$  and  $G2/G3$ . GB of  $G1/G2$  and  $G1/G3$  ( $G2/G3$ ) make a loop around two-sided  $G1$  ( $G2$ ). Opposite sums of 3  $M$  TJ132 at  $G1/G3/G2$  and in TJ231 at  $G2/G3/G1$  are:  $TJ132 = A13 + A32 + A21 = (60^\circ - A31) + (60^\circ - A23) + (60^\circ - A12) = 180^\circ - A23 - A31 - A12 = 180^\circ - TJ231$  in analogy to a simplest chirality of reflected triangles. The most stable are TJ with all 3 GB  $15^\circ < M < 30^\circ$  or  $45^\circ > M > 30^\circ$ , the best if all near  $20^\circ$  or near  $40^\circ$ . For GB  $30^\circ$  some from other two GB in TJ with  $60^\circ$  must be unstable with  $\leq 30^\circ/2$ , or in TJ  $120^\circ$  with  $\geq 90^\circ/2$ . For GBs with both TJ of the same kind, some GB from nearest four, like vertical lines in letter H with horizontal GBs, must have low angle ( $\leq 15^\circ$  TJ  $60^\circ$  or  $\geq 45^\circ$  TJ  $120^\circ$ ) and often easily disperse into 5/7. The even-sided (2,4,6,8...) grains with an opposite alternating consecutive TJ are more possible, but are rare because then grain growth involves the same kind GBs. Also a direct observation of simulated 2D 5H7 polycrystal exhibits only two possible TJ with additional disclination 5 for  $60^\circ$  or 7 for  $120^\circ$ . Topological charge of disclination is screened by an opposite nearest disclination of dislocation in three GB. Extremely high-angle ( $\sim 30^\circ$ ) GBh splits at TJ into two low-angle GB. In such cases the central 5 or 7 in TJ is GBh last disclination closest to opposite nearest disclination of dislocation in other GB. Boris Yakobson [2] exhibits alternating TJ of  $30^\circ$  GBh: 7 in Fig1 and 5 in Fig2. In TJ with two coincident GB1 and GB2, the third GB3 must be also coincident. If sigma  $s1$  and  $s2$  are Eisenstein primes  $1+3\cdot n$  [3], then GB3 sigma  $s3 = s1 \cdot s2$ . Eisenstein primes are stochastic if Riemann hypothesis is true, have angular equal distribution and other very significant meanings. In 2D polycrystal of grains with square lattice, Gaussian primes  $1+4\cdot n$  are main sigma of coincident GB. Existence of only two alternating TJ of GB could be proven for grains with any 2D lattice in a way similar to above proofs. Affordable colorful animation clips could present: the movements of thought-provoking TJ of GB with sigma = 7, 13, 19, 31, 37, 43, 49, 91, 133 ... and TJ with not coincident GB; the transformation of GB with partial disclinations [4] changing a misorientation shown so often in enclosed frame; the recrystallization of 2D polycrystal with many GB, TJ, 5/7 edge dislocations, disclinations, vacancies, interstitials, 5H7 ... Delaunay triangulation dual to simulated centroidal Voronoi polygons enables a perception of anisotropy and enhances deformation strain of 5H7. A saturated colors circle represents the angles (modulo  $60^\circ$ ) of neighbors bonds, so that bonds of equilateral triangle have the same color. One color abounds in grain. Analyzing of such interactive dynamical rearrangement enables better understanding of 2D polycrystal.

## References

- [1] L.P. Biró and P. Lambin, New Journal of Physics, **15/3** (2013) 035024.
- [2] Z. Song, V.I. Artyukhov, B.I. Yakobson and Z. Xu, Nano Letters, **13/4** (2013) 1829.
- [3] M. Baake and U. Grimm, Zeitschrift für Kristallographie, **221/8** (2006) 571.
- [4] I.A. Ovidko, Reviews on Advanced Materials Science, **30/3** (2012) 201.



Two alternating TJ of boundary between blue (G1) and red (G2) grains at left. Try both greens as big G3