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NANOTWIN GOVERNED TOUGHENING MECHANISM IN HIERARCHICALLY STRUCTURED MATERIALS

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As an important class of natural biocomposite materials, mollusk shells possess remarkable mechanical strength and toughness as a consequence of their hierarchical structuring of soft organic and hard mineral constituents through biomineralization. *Strombus gigas,* one of the toughest mollusk shell (99 wt% $CaCO_3$, 1 wt% organic), contains high density of nanoscale {110} growth twins in its third order lamellae, the basic building block of the material [1]. Although the existence of these nanotwins has been known for decades their roles and functions in mechanical behaviors and properties of biological materials are still unrevealed because numerous studies in recent years aimed to investigate the relationship between mechanical properties and the elegant nano- and hierarchical structures[1-2]. To evaluate the actual role of these nanotwins, we performed *in situ* TEM deformation experiment, large scale atomistic simulations and finite element modeling. With these analytic tools, we revealed nano scale twins in conch shell provide a basis of the several orders higher toughness comparing to twin free aragonite. In terms of qualitative experiment, we observed nanotwins can hinder crack propagation effectively comparing to twin free single crystal aragonite and leaving phase transformed area near crack tip (Fig 1 a-c) by *in situ* TEM deformation experiment. Through large scale MD simulation, we confirmed this phase transformation as a hitherto unknown toughening mechanism governed by nanoscale twins. For the quantitative comparison in terms of toughness, we performed specially designed *in situ* TEM experiments additionally for conch shell and aragonite single crystal so as to assess the contributions of these nanoscale twins on toughness of conch shell (Fig 1.d). By combining *in situ* TEM nanoscale mechanical test and FEM simulation, we found that nanotwins in 3rd order lamellar can increase fracture energy an order magnitude higher than twin free aragonite and this effect become amplified via structural hierarchy. The unique properties and structural features of nanotwinned aragonitic conch shell are expected to provide a guide to designing and fabricating hierarchically structured biomimetic materials with high toughness and high modulus.

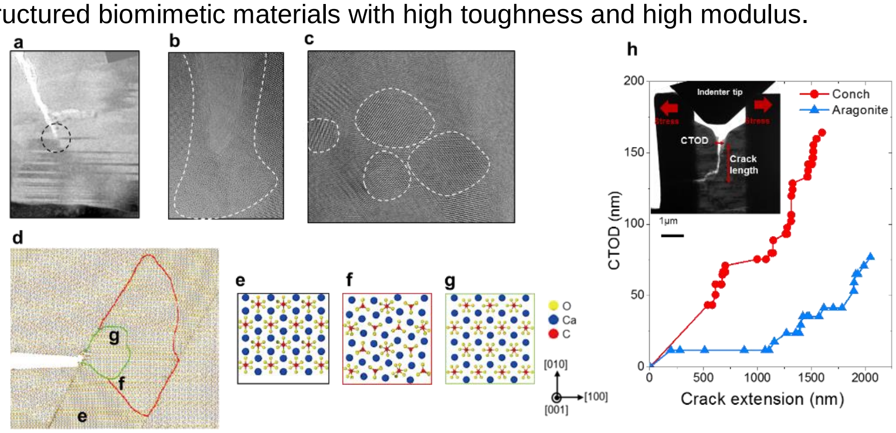

Figure 1 *(a) Crack tip hindrance at twin boundary in conch shell. (b) Phase transformation and (c) nanograin formation around crack tip from dotted circle in a. (d) Atomistic simulation of crack tip structural transformation by twin boundary. (e) Atomic configuration of untransformed region. (f-g) Atomic configuration of transformed region as a result of CO3 group rotation. (h) CTOD vs Crack extension plot of conch and single crystal aragonite from in situ TEM nanoscale mechanical test results. Inset shows specimen design used in the test.*

[1] Kamat, S. et al., Structural basis for the fracture toughness of the shell of the conch Strombus gigas. *Nature* **405**, 1036 (2000)
[2] Ortiz, C et al., Bioinspired structural materials. *Science* **319**, 1053 (2008)