

# Structure-Properties-Correlation of Cross-Linked Penicillin G Acylase Crystals

Marta Kubiak <sup>1,\*</sup>, Janine Mayer <sup>2,\*</sup>, Ingo Kampen <sup>1</sup>, Carsten Schilde <sup>1</sup> and Rebekka Biedendieck <sup>2,\*</sup>

Table S1: Summary of mechanical properties of CLECs

Enzyme crystal	Specifics	Measuring method	Results / MPa		Literature
			Hardness	Young's modulus	
Lysozyme	Native, wet tetragonal crystals	micro-Vickers hardness	2 - 20	-	[10,11,13]
Lysozyme	Native, wet orthorombic crystals	micro-Vickers hardness	6 - 10	-	[12]
Lysozyme	Native, wet tetragonal crystals	Nanoindenter	15	490	[14]
Lysozyme	Native, dry tetragonal crystals	Nanoindenter	200	4200	[14]
Lysozyme	Cross-linked triclinic crystals	mechanical resonance technique	-	290 - 1400	[15]
Lysozyme	Cross-linked tetragonal crystals in liquid	AFM Nanoindentation	11	1000	[16]
HheG	Cross-linked hexagonal crystals in liquid	AFM Nanoindentation	9	500	[16]
HheG	Cross-linked anisotropic crystal faces	AFM Nanoindentation	Vary with the cross-linking time		[17]

## References (Numbered according to the main paper):

10. Koizumi, H.; Kawamoto, H.; Tachibana, M.; Kojima, K. Effect of intracrystalline water on micro-Vickers hardness in tetragonal hen egg-white lysozyme single crystals. *J. Phys. D. Appl. Phys.* **2008**, *41*, 074019.
11. Tachibana, M.; Kobayashi, Y.; Shimazu, T.; Ataka, M.; Kojima, K. Growth and mechanical properties of lysozyme crystals. *J. Cryst. Growth* **1999**, *198–199*, 661–664.
12. Suzuki, R.; Kishi, T.; Tsukashima, S.; Tachibana, M.; Wako, K.; Kojima, K. Hardness and slip systems of orthorhombic hen egg-white lysozyme crystals. *Philos. Mag.* **2016**, *96*, 2930–2942.
13. Kishi, T.; Suzuki, R.; Shigemoto, C.; Murata, H.; Kojima, K.; Tachibana, M. Microindentation Hardness of Protein Crystals under Controlled Relative Humidity. *Crystals* **2017**, *7*, 339.
14. Tait, S.; White, E.T.; Litster, J.D. Mechanical Characterization of Protein Crystals. *Part. Part. Syst. Charact.* **2008**, *25*, 266–276.
15. Morozov, V.N.; Morozova, T.Y. Viscoelastic properties of protein crystals: Triclinic crystals of

- hen egg white lysozyme in different conditions. *Biopolymers* **1981**, *20*, 451–467.
16. Kubiak, M.; Solarczek, J.; Kampen, I.; Schallmey, A.; Kwade, A.; Schilde, C. Micromechanics of anisotropic cross-linked enzyme crystals. *Cryst. Growth Des.* **2018**, *18*, 5885–5895.
17. Kubiak, M.; Storm, K.F.; Kampen, I.; Schilde, C. Relationship between Cross-Linking Reaction Time and Anisotropic Mechanical Behavior of Enzyme Crystals. *Cryst. Growth Des.* **2019**, *19*, 4453–4464.