

METASET Results: Level-Set Functions of Diverse 3D Metamaterial Families

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The level-set functions are derived based on Shmueli, U., 2010. *International Tables for Crystallography: Volume B, Reciprocal space*. pp.156-161.

Please cite our work:

[1] Chan, Y.-C., Ahmed, F., Wang, L., and Chen, W., 2020. "METASET: Exploring Shape and Property Spaces for Data-Driven Metamaterials Design." <https://arxiv.org/abs/2006.02142>. (Preprint submitted to *Journal of Mechanical Design*).

[2] Chan, Y.-C., Ahmed, F., Wang, L., and Chen, W., 2020. "METASET: An Automated Data Selection Method for Scalable Data-Driven Design of Metamaterials." *ASME 2020 International Design Engineering Technical Conferences*.

Data availability: <https://github.com/lychan110/metaset>

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Notation:

- ❖ $x = 2\pi X, y = 2\pi Y, z = 2\pi Z; X, Y, Z \in [0,1]$
- ❖ $c x = \cos x, c y = \cos y, c z = \cos z$
- ❖ $s x = \sin x, s y = \sin y, s z = \sin z$
- ❖ $c 2x = \cos 2x$, etc.
- ❖ $s 2x = \sin 2x$, etc.
- ❖ t is a density control parameter
- ❖ The space group, origin, A/B and (hkl) information used to derive the level-set functions are also provided.

Shape Diverse (S10) Set

Space Group	Origin	A/B	(hkl)	Level-Set Function
195	1	A	(001)	$cx + cy + cz \leq t$
218	1	A	(011)	$2(cx \cdot cy + cx \cdot cz + cy \cdot cz) \geq t$
222	2	A	(011)	$2(sx \cdot sy + sx \cdot sz + sy \cdot sz) \leq t$
213	1	B	(011)	$2(sx \cdot cy + cx \cdot sz + sy \cdot cz) \geq t$
214	1	B	(011)	$2(sx \cdot cy + cx \cdot sz + sy \cdot cz) \leq t$
210	1	B	(001)	$-cx - cy - cz \leq t$
213	1	B	(122)	$cx(c^2y \cdot s^2z + s^2y \cdot s^2z) + cy(s^2x \cdot c^2z + s^2x \cdot s^2z) + cz(c^2x \cdot s^2y + s^2x \cdot s^2y) \leq t$
203	2	A	(111)	$3(cx \cdot cy \cdot cz + cx \cdot sy \cdot sz + sx \cdot cy \cdot sz + sx \cdot sy \cdot cz) \geq t$
203	2	A	(111)	$3(cx \cdot cy \cdot cz + cx \cdot sy \cdot sz + sx \cdot cy \cdot sz + sx \cdot sy \cdot cz) \leq t$
222	2	B	(011)	$[2(sx \cdot sy + sx \cdot sz + sy \cdot sz)]^2 \leq t^2$

* Complementary functions highlighted in the same color

Shape and Property (SP10) Diverse Set

Space Group	Origin	A/B	(hkl)	Level-Set Function
195	1	A	(001)	$cx + cy + cz \leq t$
198	1	A	(222)	$3c^2x \cdot c^2y \cdot c^2z \leq t$
226	1	A	(012)	$cx(c^2y - c^2z) + cy(c^2z - c^2x) + cz(c^2x - c^2y) \geq t$
217	1	A	(001)	$2(cx + cy + cz) \geq t$
213	1	B	(122)	$cx(c^2y \cdot s^2z + s^2y \cdot s^2z) + cy(s^2x \cdot c^2z + s^2x \cdot s^2z) + cz(c^2x \cdot s^2y + s^2x \cdot s^2y) \leq t$
222	2	B	(011)	$2(sx \cdot sy + sx \cdot sz + sy \cdot sz) \leq t$
203	2	A	(111)	$3(cx \cdot cy \cdot cz + cx \cdot sy \cdot sz + sx \cdot cy \cdot sz + sx \cdot sy \cdot cz) \geq t$
202	1	A	(011)	$2(cx \cdot cy + cx \cdot cz + cy \cdot cz) \leq t$
213	1	B	(011)	$2(sx \cdot cy + cx \cdot sz + sy \cdot cz) \geq t$
201	2	A	(112)	$2(c^2x \cdot sy \cdot sz + sx \cdot c^2y \cdot sz + sx \cdot sy \cdot c^2z) \leq t$

* Complementary functions highlighted in the same color

Property Diverse (P10) Set

Space Group	Origin	A/B	(hkl)	Level-Set Function
195	1	A	(001)	$cx + cy + cz \leq t$
195	1	A	(111)	$[3(cx \cdot cy \cdot cz)]^2 \leq t^2$
195	1	A	(112)	$cx \cdot c2y \cdot c2z + c2x \cdot cy \cdot c2z + c2x \cdot c2y \cdot cz \geq t$
195	1	A	(001)	$cx + cy + cz \geq t$
213	1	B	(122)	$cx(c2y \cdot s2z + s2y \cdot s2z) + cy(s2x \cdot c2z + s2x \cdot s2z) + cz(c2x \cdot s2y + s2x \cdot s2y) \leq t$
207	1	A	(012)	$cx(c2y + c2z) + cy(c2x + c2z) + cz(c2x + c2y) \leq t$
195	1	A	(001)	$[cx + cy + cz]^2 \leq t^2$
227	1	A	(111)	$6(cx \cdot cy \cdot cz + sx \cdot sy \cdot sz) \leq t$
203	1	A	(122)	$cx \cdot c2y \cdot c2z + c2x \cdot cy \cdot c2z + c2x \cdot c2y \cdot cz - sx \cdot s2y \cdot s2z - s2x \cdot sy \cdot s2z - s2x \cdot s2y \cdot sz \leq t$
213	1	B	(122)	$cx(c2y \cdot s2z + s2y \cdot s2z) + cy(s2x \cdot c2z + s2x \cdot s2z) + cz(c2x \cdot s2y + s2x \cdot s2y) \geq t$

* Complementary functions highlighted in the same color