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Supporting information for article:

Stress-induced detwinning and martensite transformation in an austenite Ni–Mn–Ga alloy with martensite cluster under uniaxial loading

Long Hou, Ying Niu, Yanchao Dai, Lansong Ba, Yves Fautrelle, Zongbin Li, Bo Yang, Claude Esling and Xi Li
Table S1  Minimum misorientation angle and the two near-180° misorientation angles, with their corresponding rotation axes, between the intra-plate major and minor twinning variants shown in Fig. 3; for each misorientation angle $\omega$, there is a family of eight equivalent rotations with eight corresponding equivalent axes $d$, which transform into each other according to the tetragonal rotation symmetry group.

| Variant pairs          | Misorientation angle $\omega$ (°) | Rotation axis, $d$ |  
|------------------------|-----------------------------------|-------------------|
|                        |                                   | $d_1$  | $d_2$  | $d_3$  |  
| Intra-plate nanotwins  | 80.28                             | 0.7040 | 0.7102 | 0.0077 | 0.51° from (110)$_{Tetr}$  
|                        | 179.68                            | 0.5370 | 0.5441 | 0.6446 | 0.45° from the normal of (112)$_{Tetr}$  
|                        | 179.43                            | 0.4578 | 0.4538 | 0.7645 | 0.38° from (111)$_{Tetr}$  
|                        | 81.84                             | 0.7112 | 0.7030 | 0.0010 | 0.34° from (110)$_{Tetr}$  
|                        | 179.56                            | 0.5347 | 0.5339 | 0.6550 | 1.13° from the normal of (112)$_{Tetr}$  
|                        | 179.93                            | 0.4605 | 0.4658 | 0.7556 | 1.15° from (111)$_{Tetr}$  
| Inter-plate major-major| 83.64                             | 0.6997 | 0.7123 | 0.0555 | 3.22° from (110)$_{Tetr}$  
|                        | 179.32                            | 0.5532 | 0.5008 | 0.6657 | 2.90° from the normal of (112)$_{Tetr}$  
|                        | 175.76                            | 0.4669 | 0.4753 | 0.7458 | 2.01° from (111)$_{Tetr}$  
| Inter-plate minor-minor| 9.74                              | 0.7566 | 0.0452 | 0.6523 | 11.55° from (301)$_{Tetr}$ Or 2.63° from (201)$_{Tetr}$  
|                        | 175.11                            | 0.7444 | 0.6660 | 0.0482 | 4.21° from the normal of (110)$_{Tetr}$  
|                        | 179.56                            | 0.0554 | 0.9964 | 0.0642 | 4.86° from (010)$_{Tetr}$  
|                        | 82.87                             | 0.7100 | 0.7042 | 0.0050 | 0.37° from (110)$_{Tetr}$  
|                        | 179.69                            | 0.5325 | 0.5278 | 0.6618 | 1.66° from the normal of (112)$_{Tetr}$  
|                        | 179.62                            | 0.4660 | 0.4699 | 0.7497 | 1.65° from (111)$_{Tetr}$  
|                        | 81.47                             | 0.7089 | 0.7053 | 0.0038 | 0.26° from (110)$_{Tetr}$  
|                        | 179.81                            | 0.5375 | 0.5340 | 0.6526 | 0.96° from the normal of (112)$_{Tetr}$  
|                        | 179.72                            | 0.4602 | 0.4626 | 0.7577 | 0.95° from (111)$_{Tetr}$  

| Inter-plate       | \( V_δ/V_γ \) | \( V_δ/V_δ \) | \( V_δ/V_δ \) | \( V_δ/V_δ \) |
|-------------------|----------------|----------------|----------------|----------------|
| major-major       | 84.37          | 0.7017         | 0.7101         | 0.0575         | 3.31° from \( \langle 110 \rangle_{\text{Tetr}} \) |
|                   | 179.54         | 0.5513         | 0.4966         | 0.6704         | 3.23° from the normal of \( \langle 112 \rangle_{\text{Tetr}} \) |
|                   | 175.57         | 0.4772         | 0.4716         | 0.7415         | 2.36° from \( \langle 111 \rangle_{\text{Tetr}} \) |
| minor-minor       | 8.53           | 0.7114         | 0.0779         | 0.6984         | 15.6° from \( \langle 301 \rangle_{\text{Tetr}} \) |
|                   | 176.18         | 0.7423         | 0.6688         | 0.0415         | Or 6.08° from \( \langle 201 \rangle_{\text{Tetr}} \) |
|                   | 179.34         | 0.0519         | 0.9973         | 0.0529         | 3.81° from the normal of \( \langle 110 \rangle_{\text{Tetr}} \) |
|                   |                |                |                |                | 4.25° from \( \langle 010 \rangle_{\text{Tetr}} \) |
Table S2  The deformation gradient tensors $M$ of the theoretically calculated martensite variants under the N-W relationship in the crystal coordinate system.

| Variant type | Deformation gradient tensor, $\varepsilon_{ij}$ |
|--------------|-----------------------------------------------|
| $V_1$        | 0.9336 -0.0016 -0.0660                        |
|              | -0.0016 0.9336 -0.0660                        |
|              | 0.0550 0.0550 1.1189                          |
| $V_2$        | 1.1189 0.0550 0.0550                          |
|              | -0.0660 0.9336 -0.0016                        |
|              | -0.0660 -0.0016 0.9336                        |
| $V_3$        | 1.1189 0.0550 -0.0550                         |
|              | -0.0660 0.9336 0.0016                         |
|              | 0.0660 0.0016 0.9336                          |
| $V_4$        | 0.9336 0.0016 -0.0660                         |
|              | 0.0016 0.9336 0.0660                          |
|              | 0.0550 -0.0550 1.1189                         |
| $V_5$        | 1.1189 -0.0550 -0.0550                        |
|              | 0.0660 0.9336 -0.0016                         |
|              | 0.0660 -0.0016 0.9336                         |
| $V_6$        | 0.9336 -0.0660 0.0016                         |
|              | 0.0550 1.1189 -0.0550                         |
|              | 0.0016 0.0660 0.9336                          |
| $V_7$        | 0.9336 0.0016 0.0660                          |
|              | 0.0016 0.9336 -0.0660                         |
|              | -0.0550 0.0550 1.1189                         |
| $V_8$        | 0.9336 0.0660 -0.0016                         |
|              | -0.0550 1.1189 -0.0550                         |
|              | -0.0016 0.0660 0.9336                         |
| $V_9$        | 1.1189 -0.0550 0.0550                         |
|              | 0.0660 0.9336 0.0016                          |
|              | -0.0660 0.0016 0.9336                         |
| $V_{10}$     | 0.9336 -0.0016 0.0660                          |
|              | -0.0016 0.9336 0.0660                          |
|              | -0.0550 -0.0550 1.1189                         |
| $V_{11}$     | 0.9336 0.0660 0.0016                          |
|              | -0.0550 1.1189 0.0550                          |
**Table S3**  The deformation gradient tensors $\mathbf{M}$ of the theoretically calculated martensite variants under the K-S relationship in the crystal coordinate system.

| Variant type | Deformation gradient tensor, $\varepsilon_{ij}$ |
|--------------|-----------------------------------------------|
| $V_1$        | 0.9310 0.0262 -0.1023                         |
|              | -0.0285 0.9345 -0.0285                         |
|              | 0.0845 0.0262 1.1177                           |
| $V_2$        | 1.1177 0.0262 0.0845                           |
|              | -0.0285 0.9345 -0.0285                         |
|              | -0.1023 0.0262 0.9310                          |
| $V_3$        | 1.1177 0.0262 -0.0845                          |
|              | -0.0285 0.9345 0.0285                          |
|              | 0.1023 -0.0262 0.9310                          |
| $V_4$        | 0.9310 -0.0262 -0.1023                         |
|              | 0.0285 0.9345 0.0285                           |
|              | 0.0845 -0.0262 1.1177                          |
| $V_5$        | 1.1177 -0.0262 -0.0845                         |
|              | 0.0285 0.9345 -0.0285                          |
|              | 0.1023 0.0262 0.9310                           |
| $V_6$        | 0.9310 -0.1023 -0.0262                         |
|              | 0.0845 1.1177 -0.0262                          |
|              | 0.0285 0.0285 0.9345                           |
| $V_7$        | 0.9310 -0.0262 0.1023                          |
|              | 0.0285 0.9345 -0.0285                          |
|              | -0.0845 0.0262 1.1177                          |
| $V_8$        | 0.9310 0.1023 0.0262                           |
|              | -0.0845 1.1177 -0.0262                         |
|              | -0.0285 0.0285 0.9345                          |
|   | V_9    | V_10   | V_11   | V_12   | V_13   | V_14   | V_15   | V_16   | V_17   | V_18   | V_19   | V_20   |
|---|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| V_9 | -0.0262 | 0.9310 | 0.1023 | 1.1177 |
| V_10| 0.0262  | -0.0845| 0.1023 | 1.1177 |
| V_11| -0.0285 | 0.9345 | 0.0285 | 0.9345 |
| V_12| -0.0262 | -0.0845| -0.0285| 0.9345 |
| V_13| 0.0262  | 1.1177 | 0.9310 | 0.9310 |
| V_14| 0.0262  | -0.0285| -0.0285| 0.9345 |
| V_15| 1.1177  | 0.0845 | -0.0262| 0.9345 |
| V_16| -0.1023 | 0.9310 | -0.0262| 0.9345 |
| V_17| 0.0262  | 1.1177 | 0.0845 | 0.9345 |
| V_18| 0.0262  | -0.0262| -0.1023| 0.9310 |
| V_19| 0.0262  | 1.1177 | -0.0845| 0.9310 |
| V_20| 0.0262  | -0.0262| -0.0845| 1.1177 |
| Variant pair | Deformation gradient tensor, $\varepsilon_{ij}$ |
|--------------|-----------------------------------------------|
| Plate A      | 1.0486 0.0038 0.0442 |
|              | 0.0097 1.0024 -0.0088 |
|              | -0.0520 0.0117 0.9339 |
| Plate B      | 0.9339 -0.0117 -0.0520 |
|              | 0.0088 1.0024 -0.0097 |
|              | 0.0442 -0.0038 1.0486 |

**Table S4** The deformation gradient tensors $M$ of the variant combination in Plate A and Plate B, as illustrated in Fig. 2, in the crystal coordinate system.
Figure S1. Demonstration of different possible orientation relationships between austenite and martensite, and corresponding pole figures. (a) Bain relation: \((001)_A/(001)_M, [100]_A/[1-10]_M\); (b) K-S relation: \((111)_A/(101)_M, [1-10]_A/[11-1]_M\); (c) N-W relation: \((111)_A/(101)_M, [-211]_A/[10-1]_M\); (d) Pitsch relation: \((110)_A/(1-1-2)_M, [1-10]_A/[1-11]_M\). The common poles are enclosed with open circles. It indicates that during the martensitic transformation the major variant agrees well with the N-W relationship and the minor variant agrees with the K-S relationship.