

Supporting information

for

The Preparation of a Challenging Superconductor Nb₃Al by Exploiting Nano Effect

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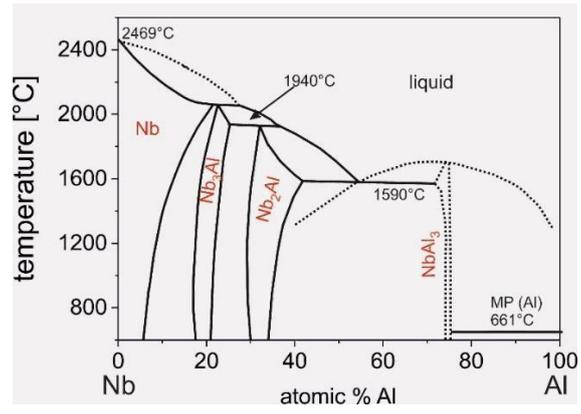


Figure S1 Reproduction of the Nb Al phase diagram according to ref. [1].

S2. X-ray powder diffraction of Nb₃Al samples

XRD patterns of Nb₃Al samples were plotted in **Figure S2-S3**. In **Figure S2**, the samples were sintered at 1400°C with ratios of Nb_p:Al ranging from 2.8:1 to 3.6:1. The reaction times were 6h and 16h for the two series((a) and (b)). In **Figure S3**, the samples were sintered at 1350°C with ratios of Nb_p:Al ranging from 2.8:1 to 3.2:1. Here, the reaction times were 6h, 20h and 21h, respectively. All samples were sintered under a mixture of hydrogen and argon atmosphere with 5% hydrogen concentration.

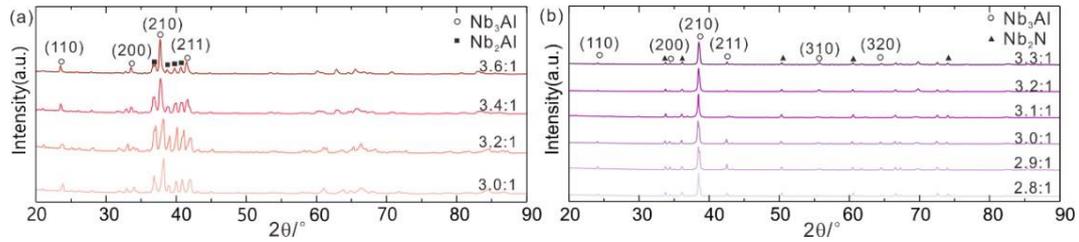


Figure S2 XRD patterns of samples prepared at 1400 °C with various sintering time and compositions (a) 6h (Nb_p:Al = 3.0:1, 3.2:1, 3.4:1, 3.6:1); (b) 16h (Nb_p:Al = 2.8:1, 2.9:1, 3.0:1, 3.1:1, 3.2:1, 3.3:1).

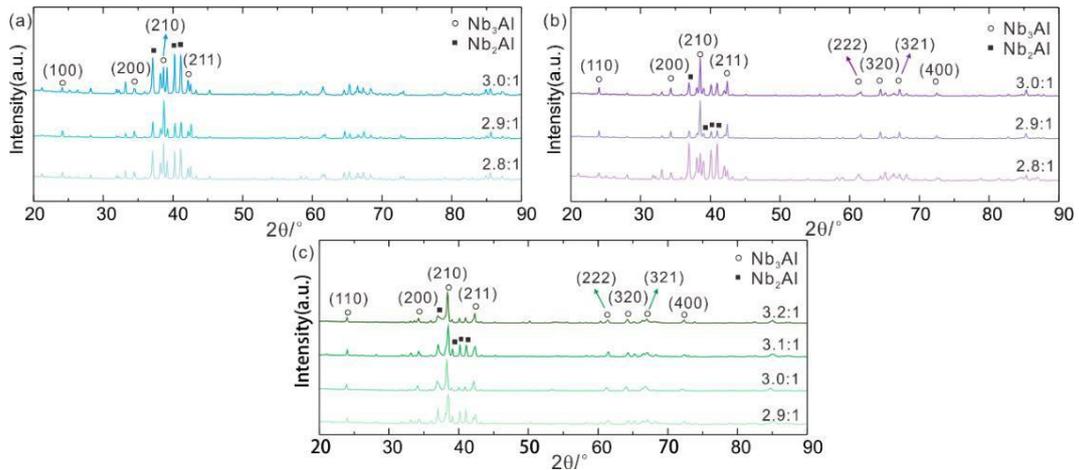


Figure S3 XRD patterns of samples prepared at 1350 °C with various sintering time and compositions (a) 6h (Nb_p:Al = 2.8:1, 2.9:1, 3.0:1); (b) 20h (Nb_p:Al = 2.8:1, 2.9:1, 3.0:1); (c) 21h (Nb_p:Al = 2.9:1, 3.0:1, 3.1:1, 3.2:1).

S3. SEM images of Nb₃Al samples

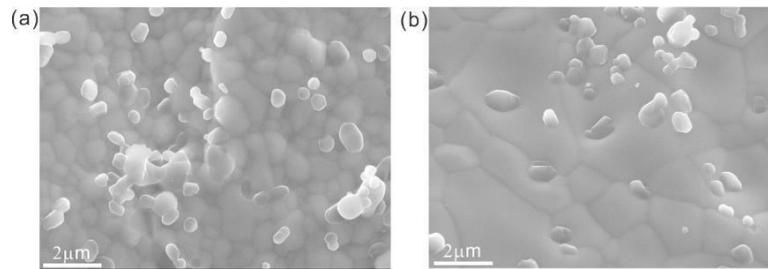


Figure S4 SEM images of Nb₃Al samples sintered at (a) 1300°C and (b) 1400°C for 10h with

Nb_p:Al = 3.0:1

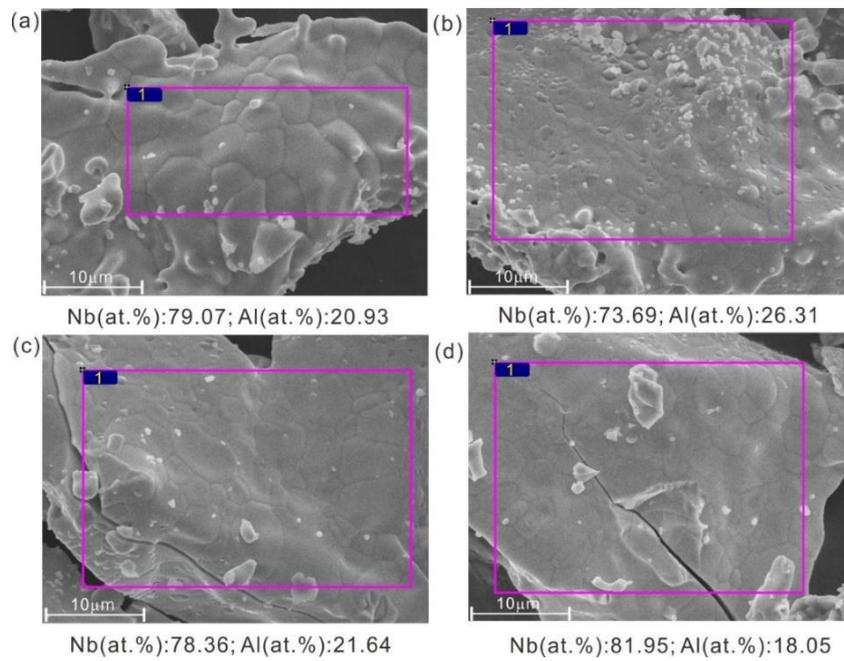


Figure S5 SEM images of Nb₃Al samples sintered at 1400°C for 10h with Nb_p: Al= (a) 2.9:1;

(b)3.0:1; (c)3.5:1; (d) 3.75:1

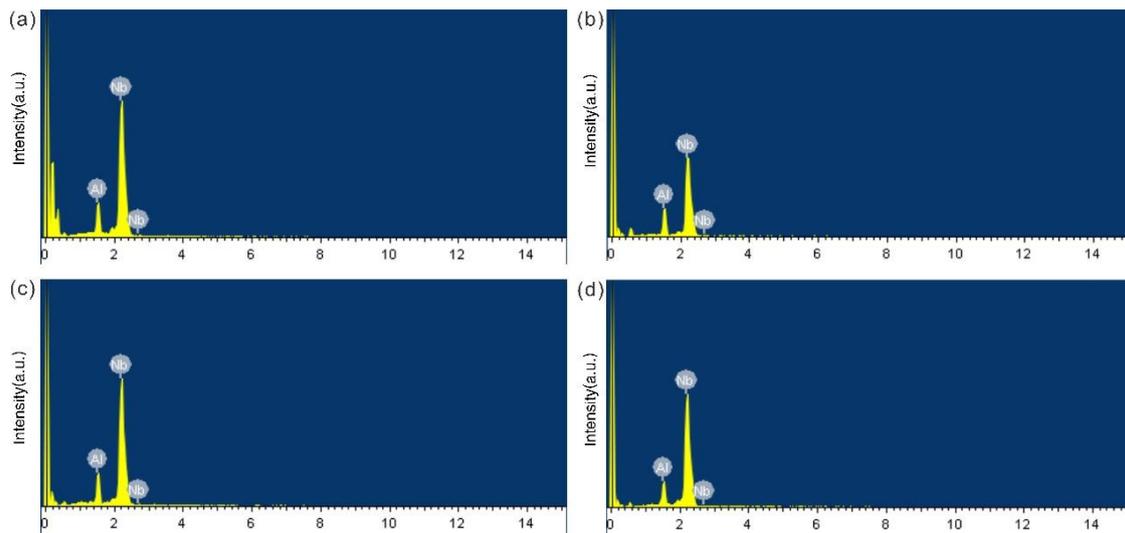


Figure S6 EDS images of Nb₃Al samples sintered at 1400°C for 10h with Nb_p: Al= (a) 2.9:1;
(b)3.0:1; (c)3.5:1; (d) 3.75:1

S4. Crystal data of Nb [2]

Space group: $Im\bar{3}m$

Lattice parameter: $a = 3.306 \text{ \AA}$

Wyckoff position and atomic position: Nb 2a, (0, 0, 0)

S5. Particle Models and Calculated Results

To understand the face, size, and shape dependence of MSE for a particle, we have designed four families of models as shown in Figure S5. Family a) contains five models built by expanding the basic unit cell of BCC Nb along the b axis, i.e. [010] direction ([uvw] indices of a lattice direction; $\langle uvw \rangle$ indices of a set of all symmetrically equivalent lattice directions; {hkl} indices of a set of all symmetrically equivalent crystal faces), each step by one unit cell length; while family b) contains ones built by a similar way as for type a) along three equivalent lattice directions simultaneously $\langle 100 \rangle$; family c) are ones built by expanding the BCC structure of Nb from a center atom along the 12 equivalent lattice directions $\langle 110 \rangle$, each step by one inter-planar spacing d_{110} ; family d) are similarly built as type c) along the eight equivalent $\langle 111 \rangle$ directions. On the left side of Figure 4 in the main text show the starting models in each type, respectively, while on the right side the second models in each type are given, respectively. In each type, we have prepared 5 models as shown in Figure 4. To calculate E_{model}^N in Eq. (4) on the same footing as E_{bulk}^N , a 3D periodic lattice model with a vacuum layer of 15 Å between the models is used. The calculated energies were used as input to calculate the MSEs, E_S , E_N , by Eq. (3) and (4), respectively. The calculated results are shown in **Table S1**.

Table S1. Total energy of a particle model with N atoms, total energy of N atoms in a bulk solid without surface and the average surface energy normalized to one atom of different models

series	structure	N	E_{Model}^N (eV)	$N \cdot \tilde{E}_{bulk}$ (eV)	E_N (eV/atom)
line	1×1×1	9	-55.173857	-90.6323445	3.939831944
	1×2×1	14	-92.564155	-140.983647	3.458535143
	1×3×1	19	-130.42635	-191.3349495	3.205715763
	1×4×1	24	-167.9992	-241.686252	3.070293833
	1×5×1	29	-205.61143	-292.0375545	2.98021119
{100}	1×1×1	9	-55.173857	-90.6323445	3.939831944
	2×2×2	35	-267.26019	-352.4591175	2.434255071
	3×3×3	91	-768.05242	-916.3937055	1.630124016
	4×4×4	189	-1676.4459	-1903.279235	1.200176373
	5×5×5	341	-3115.8097	-3433.958831	0.932988652
{110}	{110}-1	15	-120.45307	-151.0539075	2.040055833
	{110}-2	65	-576.80277	-654.5669325	1.196371731
	{110}-3	175	-1623.3315	-1762.295588	0.7940805
	{110}-4	369	-3502.5733	-3715.926125	0.578191936
	{110}-5	671	-6461.9671	-6757.144796	0.439907147

{111}	{111}-1	7	-23.861282	-70.4918235	6.661505929
	{111}-2	33	-232.26458	-332.3185965	3.031939894
	{111}-3	95	-781.10391	-956.6747475	1.848114079
	{111}-4	209	-1836.1826	-2104.684445	1.284697821
	{111}-5	391	-3781.0417	-3937.471856	0.400077124

Table S2. The calculated data used to calculate the E_S . The surface area S in the third column corresponds to the N -atom particle in Table S1. The E_{slab}^N in Eq. (3) of the main text is replaced by the E_{Model}^N .

series	structure	S (Å ²)	E_{Model}^N (eV)	$N \cdot \tilde{E}_{bulk}$ (eV)	E_S (eV/Å ²)
line	1×1×1	65.58971814	-55.173857	-90.6323445	0.270305229
	1×2×1	109.3161969	-92.564155	-140.983647	0.221465315
	1×3×1	153.0426757	-130.42635	-191.3349495	0.198992207
	1×4×1	196.7691544	-167.9992	-241.686252	0.187242386
	1×5×1	240.4956332	-205.61143	-292.0375545	0.179683355
{100}	1×1×1	65.58971814	-55.173857	-90.6323445	0.270305229
	2×2×2	262.3588726	-267.26019	-352.4591175	0.162370967
	3×3×3	590.3074633	-768.05242	-916.3937055	0.125647476
	4×4×4	1049.43549	-1676.4459	-1903.279235	0.108073977
	5×5×5	1639.742954	-3115.8097	-3433.958831	0.097011891
{110}	{110}-1	92.757784	-120.45307	-151.0539075	0.16495024
	{110}-2	371.0315312	-576.80277	-654.5669325	0.104794547
	{110}-3	834.818267	-1623.3315	-1762.295588	0.083230143
	{110}-4	1484.129299	-3502.5733	-3715.926125	0.071878112
	{110}-5	2318.9466	-6461.9671	-6757.144796	0.063644781
{111}	{111}-1	75.736483	-23.861282	-70.4918235	0.307847286

{111}-2	302.9459314	-232.26458	-332.3185965	0.165135105
{111}-3	681.628346	-781.10391	-956.6747475	0.128787805
{111}-4	1211.783726	-1836.1826	-2104.684445	0.110787857
{111}-5	1893.412071	-3781.0417	-3937.471856	0.09947968

References

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2. Roberge, R. Lattice-parameter of niobium between 4.2 and 300 k. *J. Less-Common Met.* **1975**, *40*, 161–164.