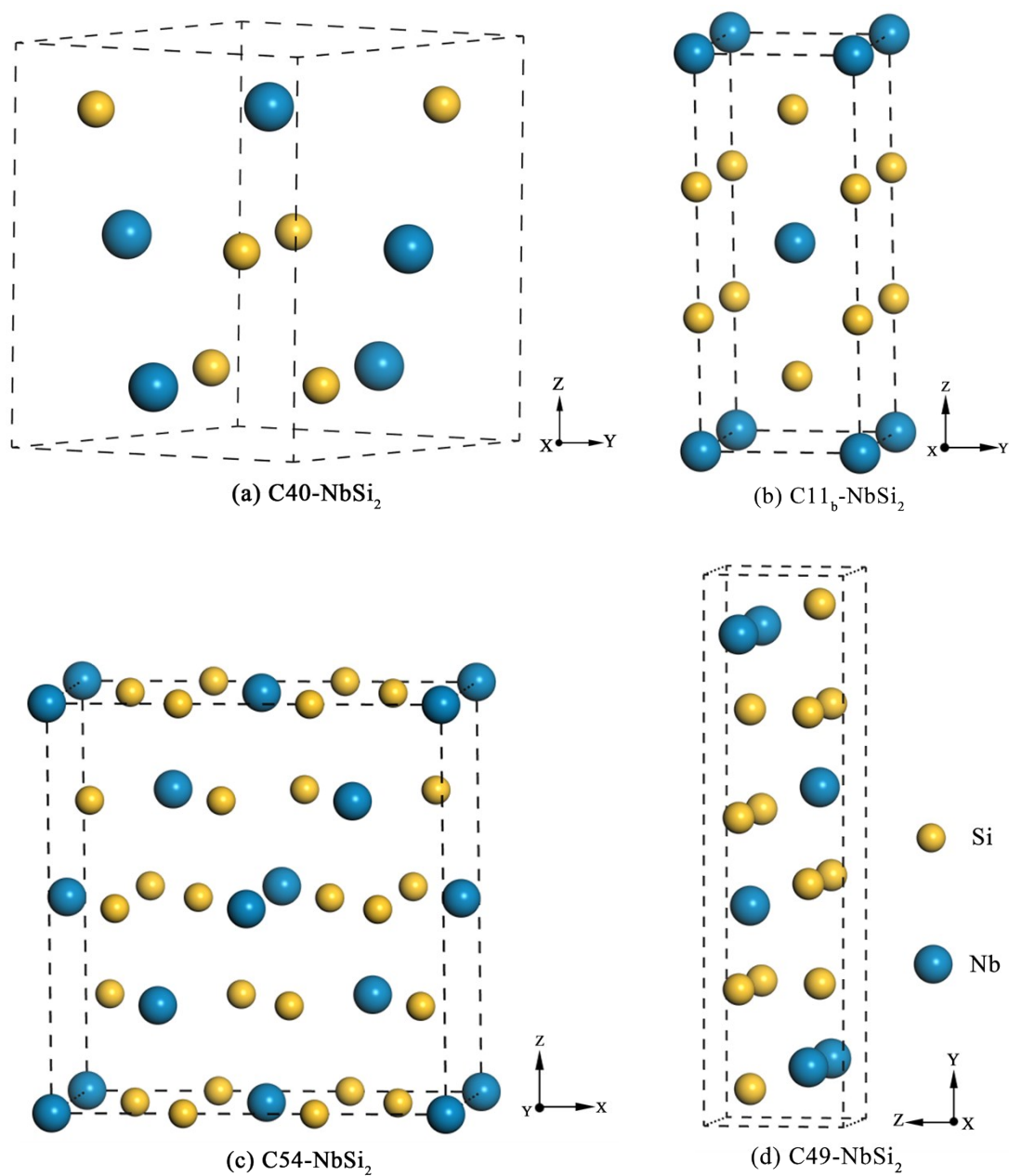


### Supporting Information:



**Fig.** The designed four crystal structures for NbSi<sub>2</sub> based on ref<sup>15-17</sup>.

15 K. Tanaka, K. Nawata, H. Inui, M. Yanmaguchi and M. Koiwa, *Intermetallics*, 2001, **9**, 603-607.

17 X. Zhang, Z. Wang and Y. Qiao, *Acta Mater.*, 2011, **59**, 5584-5592.