**Phase stability, elastic and thermodynamic properties of L12 (Co,Ni)3(Al,Mo,Nb) phase from first-principles calculations**

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1. Computational details

The atomic positions of both the 32-atom and 64-atom SQS are listed in the Table SI and Table SII, respectively. The generated 64-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb) compound is shown in Fig. S1. The correlation functions of both the 32-atom and 64-atom SQS are listed in the Table SIII and Table SIV, respectively. A 5×5×3 *k*-point mesh is used. The cutoff energy of plane wave is set as 500 eV. Convergence is judged when the energy difference between each step of the ionic iterations is less than 4×10-6 eV/atom.

2. Structural properties and elastic properties

Calculated equilibrium lattice constant and ΔH value at 0 K are summarized in Table SV. Calculated elastic properties of (Co,Ni)3(Al,Mo,Nb) at 0 K are listed in Table SVI.

Figures and Figure Captions:

FIG. S1. 64-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb).

CoNiAlMoNb64.tif

TABLE SI. Structural description of the 32-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb)

|  |
| --- |
| 7.140000000 0.000000000 0.000000000  0.000000000 7.140000000 0.000000000  0.000000000 0.000000000 7.140000000  0.000000000 0.500000000 0.000000000 Nb  0.000000000 0.000000000 0.500000000 Al  0.500000000 0.000000000 0.500000000 Al  0.000000000 0.500000000 0.500000000 Al  0.500000000 0.000000000 0.000000000 Al  0.000000000 0.000000000 0.000000000 Mo  0.500000000 0.500000000 0.000000000 Mo  0.500000000 0.500000000 0.500000000 Mo  0.500000000 0.250000000 0.250000000 Ni  0.000000000 0.750000000 0.250000000 Ni  0.500000000 0.750000000 0.250000000 Ni  0.000000000 0.250000000 0.750000000 Ni  0.750000000 0.000000000 0.250000000 Ni  0.250000000 0.500000000 0.250000000 Ni  0.750000000 0.000000000 0.750000000 Ni  0.750000000 0.500000000 0.750000000 Ni  0.250000000 0.750000000 0.000000000 Ni  0.750000000 0.750000000 0.000000000 Ni  0.750000000 0.250000000 0.500000000 Ni  0.250000000 0.750000000 0.500000000 Ni  0.000000000 0.250000000 0.250000000 Co  0.500000000 0.250000000 0.750000000 Co  0.000000000 0.750000000 0.750000000 Co  0.500000000 0.750000000 0.750000000 Co  0.250000000 0.000000000 0.250000000 Co  0.750000000 0.500000000 0.250000000 Co  0.250000000 0.000000000 0.750000000 Co  0.250000000 0.500000000 0.750000000 Co  0.250000000 0.250000000 0.000000000 Co  0.750000000 0.250000000 0.000000000 Co  0.250000000 0.250000000 0.500000000 Co  0.750000000 0.750000000 0.500000000 Co |

TABLE SII. Structural description of the 64-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb)

|  |
| --- |
| 7.1400000000 0.0000000000 0.0000000000  0.0000000000 7.1400000000 0.0000000000  0.0000000000 0.0000000000 14.280000000  0.500000000 0.000000000 0.250000000 Nb  0.500000000 0.500000000 0.750000000 Nb  0.000000000 0.000000000 0.000000000 Al  0.500000000 0.000000000 0.000000000 Al  0.500000000 0.500000000 0.000000000 Al  0.500000000 0.500000000 0.250000000 Al  0.000000000 0.000000000 0.500000000 Al  0.000000000 0.500000000 0.500000000 Al  0.500000000 0.500000000 0.500000000 Al  0.500000000 0.000000000 0.750000000 Al  0.000000000 0.500000000 0.000000000 Mo  0.000000000 0.000000000 0.250000000 Mo  0.000000000 0.500000000 0.250000000 Mo  0.500000000 0.000000000 0.500000000 Mo  0.000000000 0.000000000 0.750000000 Mo  0.000000000 0.500000000 0.750000000 Mo  0.000000000 0.250000000 0.125000000 Ni  0.500000000 0.250000000 0.125000000 Ni  0.000000000 0.250000000 0.375000000 Ni  0.000000000 0.250000000 0.625000000 Ni  0.500000000 0.250000000 0.625000000 Ni  0.000000000 0.750000000 0.375000000 Ni  0.500000000 0.250000000 0.875000000 Ni  0.500000000 0.750000000 0.875000000 Ni  0.750000000 0.500000000 0.125000000 Ni  0.250000000 0.000000000 0.375000000 Ni  0.250000000 0.000000000 0.625000000 Ni  0.750000000 0.000000000 0.625000000 Ni  0.750000000 0.500000000 0.625000000 Ni  0.250000000 0.000000000 0.875000000 Ni  0.250000000 0.500000000 0.875000000 Ni  0.750000000 0.500000000 0.875000000 Ni  0.750000000 0.250000000 0.000000000 Ni  0.250000000 0.750000000 0.000000000 Ni  0.750000000 0.750000000 0.000000000 Ni  0.250000000 0.250000000 0.250000000 Ni  0.250000000 0.750000000 0.250000000 Ni  0.750000000 0.750000000 0.250000000 Ni  0.250000000 0.750000000 0.500000000 Ni  0.750000000 0.750000000 0.750000000 Ni  0.000000000 0.750000000 0.125000000 Co  0.500000000 0.750000000 0.125000000 Co  0.500000000 0.250000000 0.375000000 Co  0.500000000 0.750000000 0.375000000 Co  0.000000000 0.750000000 0.625000000 Co  0.500000000 0.750000000 0.625000000 Co  0.000000000 0.250000000 0.875000000 Co  0.000000000 0.750000000 0.875000000 Co  0.250000000 0.000000000 0.125000000 Co  0.750000000 0.000000000 0.125000000 Co  0.250000000 0.500000000 0.125000000 Co  0.750000000 0.000000000 0.375000000 Co  0.250000000 0.500000000 0.375000000 Co  0.750000000 0.500000000 0.375000000 Co  0.250000000 0.500000000 0.625000000 Co  0.750000000 0.000000000 0.875000000 Co  0.250000000 0.250000000 0.000000000 Co  0.750000000 0.250000000 0.250000000 Co  0.250000000 0.250000000 0.500000000 Co  0.750000000 0.250000000 0.500000000 Co  0.750000000 0.750000000 0.500000000 Co  0.250000000 0.250000000 0.750000000 Co  0.750000000 0.250000000 0.750000000 Co  0.250000000 0.750000000 0.750000000 Co |

TABLE SIII. Correlation functions of the 32-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb). Let n be the number of sites it contains, let l be its diameter and let ρ be its associated correlation.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| n | l | ρ | n | l | ρ |
| 2 | 2.524371 | 0 | 3 | 5.048742 | 0.027344 |
| 2 | 2.524371 | 0 | 3 | 5.048742 | 0.011719 |
| 2 | 2.524371 | 0 | 3 | 5.048742 | 0.064275 |
| 2 | 3.57 | -0.5 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0.054127 | 3 | 5.048742 | 0.140625 |
| 2 | 3.57 | -0.109375 | 3 | 5.048742 | 0.013532 |
| 2 | 4.372339 | 0 | 3 | 5.048742 | 0.011719 |
| 2 | 4.372339 | 0 | 3 | 5.048742 | 0.010149 |
| 2 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 2 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 2 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 2 | 5.048742 | -0.1875 | 3 | 5.644666 | 0.125 |
| 2 | 5.048742 | 0.054127 | 3 | 5.644666 | -0.083333 |
| 2 | 5.048742 | -0.046875 | 3 | 5.644666 | 0 |
| 2 | 5.644666 | 0 | 3 | 5.644666 | 0 |
| 2 | 5.644666 | 0 | 3 | 5.644666 | -0.125 |
| 2 | 5.644666 | 0 | 3 | 5.644666 | 0 |
| 2 | 6.183421 | 0 | 3 | 5.644666 | 0 |
| 2 | 6.183421 | 0 | 3 | 5.644666 | -0.083333 |
| 2 | 6.183421 | -0.16238 | 3 | 5.644666 | 0 |
| 2 | 6.183421 | 0.140625 | 3 | 5.644666 | 0 |
| 2 | 6.678858 | 0 | 3 | 5.644666 | 0 |
| 2 | 6.678858 | 0 | 3 | 5.644666 | 0.072169 |
| 2 | 6.678858 | 0 | 3 | 5.644666 | 0.125 |
| 2 | 7.14 | 1 | 3 | 5.644666 | 0.072169 |
| 2 | 7.14 | 1 | 3 | 5.644666 | 0 |
| 2 | 7.14 | 0.5625 | 3 | 5.644666 | 0 |
| 2 | 7.14 | -0.16238 | 3 | 5.644666 | 0 |
| 2 | 7.14 | 0.328125 | 3 | 5.644666 | 0 |
| 3 | 2.524371 | 0 | 3 | 5.644666 | 0 |
| 3 | 2.524371 | 0 | 3 | 5.644666 | 0 |
| 3 | 2.524371 | -0.125 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0.125 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0.072169 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0.083333 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.125 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.144338 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.125 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.072169 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.125 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | -0.125 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.072169 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.083333 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | -0.083333 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.125 | 3 | 5.644666 | -0.083333 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | -0.125 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.083333 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 6.183421 | 0 |
| 3 | 4.372339 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | -0.083333 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0.083333 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0.072169 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.046875 |
| 3 | 5.048742 | -0.072169 | 3 | 6.183421 | 0.067658 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.013532 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.074219 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.067658 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | -0.082031 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.011719 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0.010149 |
| 3 | 5.048742 | 0 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0.046875 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | -0.067658 | 3 | 6.183421 | 0 |
| 3 | 5.048742 | 0.013532 | 3 | 6.183421 | 0 |

TABLE SIV. Correlation functions of the 64-atom SQS for L12 (Co,Ni)3(Al,Mo,Nb). Let n be the number of sites it contains, let l be its diameter and let ρ be its associated correlation.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| n | l | ρ | n | l | ρ |
| 2 | 2.524371 | -0.125 | 3 | 5.048742 | 0 |
| 2 | 2.524371 | 0 | 3 | 5.048742 | 0 |
| 2 | 2.524371 | 0 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0 | 3 | 5.048742 | -0.046875 |
| 2 | 3.57 | -0.046875 | 3 | 5.048742 | 0 |
| 2 | 3.57 | 0 | 3 | 5.048742 | 0.015625 |
| 2 | 3.57 | -0.03125 | 3 | 5.048742 | 0.046875 |
| 2 | 4.372339 | 0 | 3 | 5.048742 | 0.006766 |
| 2 | 4.372339 | 0 | 3 | 5.048742 | 0 |
| 2 | 4.372339 | 0.041667 | 3 | 5.048742 | 0.007813 |
| 2 | 5.048742 | -0.166667 | 3 | 5.048742 | 0.019531 |
| 2 | 5.048742 | 0 | 3 | 5.048742 | 0.037212 |
| 2 | 5.048742 | -0.09375 | 3 | 5.048742 | 0 |
| 2 | 5.048742 | 0.054127 | 3 | 5.048742 | 0 |
| 2 | 5.048742 | -0.078125 | 3 | 5.048742 | 0 |
| 2 | 5.644666 | -0.083333 | 3 | 5.048742 | 0.070313 |
| 2 | 5.644666 | 0 | 3 | 5.048742 | -0.027063 |
| 2 | 5.644666 | 0 | 3 | 5.048742 | 0.019531 |
| 2 | 6.183421 | 0 | 3 | 5.048742 | 0.050744 |
| 2 | 6.183421 | -0.140625 | 3 | 5.644666 | 0.020833 |
| 2 | 6.183421 | 0 | 3 | 5.644666 | 0.054127 |
| 2 | 6.183421 | 0 | 3 | 5.644666 | 0 |
| 2 | 6.678858 | 0.083333 | 3 | 5.644666 | 0 |
| 2 | 6.678858 | 0 | 3 | 5.644666 | 0 |
| 2 | 6.678858 | 0 | 3 | 5.644666 | -0.041667 |
| 3 | 2.524371 | 0.03125 | 3 | 5.644666 | -0.041667 |
| 3 | 2.524371 | 0.036084 | 3 | 5.644666 | 0 |
| 3 | 2.524371 | 0 | 3 | 5.644666 | 0.020833 |
| 3 | 3.57 | -0.041667 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | -0.010417 |
| 3 | 3.57 | 0.041667 | 3 | 5.644666 | -0.072169 |
| 3 | 3.57 | 0.023438 | 3 | 5.644666 | 0 |
| 3 | 3.57 | 0 | 3 | 5.644666 | 0 |
| 3 | 3.57 | -0.007813 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.0625 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | -0.018042 | 3 | 5.644666 | 0.023438 |
| 3 | 4.372339 | -0.023438 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | -0.007813 |
| 3 | 4.372339 | 0.027063 | 3 | 5.644666 | -0.026042 |
| 3 | 4.372339 | -0.007812 | 3 | 5.644666 | 0.027063 |
| 3 | 4.372339 | 0.015625 | 3 | 5.644666 | 0.005208 |
| 3 | 4.372339 | 0.045105 | 3 | 5.644666 | 0.009021 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.010417 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.036084 |
| 3 | 4.372339 | 0.020833 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | -0.054127 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | -0.072917 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.013532 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | -0.013532 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0.005208 | 3 | 5.644666 | 0.015625 |
| 3 | 4.372339 | 0.009021 | 3 | 5.644666 | 0.045105 |
| 3 | 4.372339 | 0.041667 | 3 | 5.644666 | 0.03125 |
| 3 | 4.372339 | -0.041667 | 3 | 5.644666 | 0.036084 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | -0.023438 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | -0.013532 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.013532 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0.007812 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 4.372339 | 0 | 3 | 5.644666 | 0 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0.023438 |
| 3 | 5.048742 | 0.072917 | 3 | 5.644666 | -0.013532 |
| 3 | 5.048742 | 0.036084 | 3 | 5.644666 | 0.013532 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | -0.007812 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0.041667 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0.005208 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0.009021 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | -0.041667 |
| 3 | 5.048742 | 0 | 3 | 5.644666 | 0 |

TABLE SV. Calculated equilibrium lattice constant a (nm) and enthalpy of formation ΔH (kJ/mol-atom) for 64-atom (Co,Ni)3(Al,Mo,Nb).

|  |  |  |
| --- | --- | --- |
|  | Lattice constant a | enthalpy of formation ΔH |
| (Co,Ni)3(Al,Mo,Nb) | 0.3595 | -20.45 |

TABLE SVI. Calculated elastic properties, including *C*ij, *B*, *G* and *E*, *B*/*G*, Cauchy pressure *C*12-*C*44 for 64-atom (Co,Ni)3(Al,Mo,Nb). The unit of elastic properties is GPa.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | *C*11 | *C*12 | *C*44 | *B* | *G* | *E* | *B*/*G* | *C*12-*C*44 |
| (Co,Ni)3(Al,Mo,Nb) | 286.3 | 168.9 | 147.1 | 208.0 | 101.8 | 262.5 | 2.04 | 21.8 |

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