Molecular Dynamics Study on Structural and Atomic Evolution between Au and Ni Nanoparticles through Coalescence

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Table S1. The illustration of the radius for different NPs

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | NP1 | NP2 | NP3 | NP4 |
| Au radius (nm) | **1.50** | **2.50** | **3.20** | **4.60** |
| Ni radius (nm) | **2.9** | | | |
| Atomic ratio | Au0.01Ni0.99 | Au0.05Ni0.95 | Au0.1Ni0.9 | Au0.25Ni0.75 |
|  | **NP5** | **NP6** | **NP7** | **NP8** |
| Au radius (nm) | **5.80** | **6.64** | **7.62** | **9.60** |
| Atomic ratio | Au04Ni0.6 | Au0.5Ni0.5 | Au0.6Ni0.4 | Au0.75Ni0.25 |
| Ni radius (nm) | **2.9** | | | |



Fig. S1 PDF of Au atoms and Ni atoms at temperatures 0.1 K

Table S2 Five representative temperatures (K) of NP1-NP8 during the heating process

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sample | T1 | T2 | T3 | T4 | T5 |
| NP1 | 97 | 960 | 1300 | 1401 | 1453 |
| NP2 | 288 | 960 | 1022 | 1423 | 1438 |
| NP3 | 300 | 922 | 1047 | 1380 | 1425 |
| NP4 | 464 | 712 | 1034 | 1340 | 1387 |
| NP5 | 558 | 907 | 1112 | 1271 | 1372 |
| NP6 | 477 | 874 | 1142 | 1281 | 1410 |
| NP7 | 247 | 1067 | 1142 | 1276 | 1452 |
| NP8 | 449 | 1087 | 1173 | 1319 | 1473 |



Fig. S2 MSD of Ni and Au atoms in (a) NP1, (b) NP2, (c) NP3, (d) NP4, (e) NP5, (f) NP6, (g) NP7, (h) NP8 during heating process.



Fig. S3. Snapshots at different temperatures during the coalescence, Au and Ni atoms are colored in yellow and gray, respectively.