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July 13, 2005

Abstract

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from which the activation enthalpy ΔH , activation volume ΔV , and pre-exponential factor D_0 was determined, separately for the x -, the y -, and the z -directions. The values are given in Table 1. All diffusion measurements were carried out with samples of about 3000 atoms in six double layers, and ran over 2ns (2 million time steps).

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Table 1: Activation enthalpies, activation volumes, and pre-exponential factors for diffusion in decagonal Al-Ni-Co.

Sample	Ni-rich	Ni-rich	Ni-rich	Co-rich	Co-rich	Co-rich
Atom, potential	Al, EAM	Ni, EAM	Al, pair	Al, EAM	Ni, EAM	Al, pair
ΔH_x [eV]	0.70	0.98	0.89	0.83	0.93	0.63
ΔH_z [eV]	0.58	1.11	0.64	0.83	0.97	0.66
ΔV_x [Ω]	0.11	0.17	0.17	0.14	-	0.24
ΔV_z [Ω]	0.11	0.27	0.28	0.14	-	0.33
D_{0x} [m^2/s]	6.5×10^{-8}	5.1×10^{-8}	1.8×10^{-7}	1.2×10^{-7}	1.8×10^{-8}	3.1×10^{-8}
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Figure 1: Diffusion processes in the decagonal plane (Al-Ni-Co, Ni-rich). Dark grey, large: Ni; light grey, large: Co; dark grey, small: Al initial positions; light grey, small: Al positions after 100ps. Initial and final positions are connected. Dashed lines mark supertiles. Dotted circles mark three types of decagonal clusters, differing in the Ni content.

Figure 2: Atom density maps of a supertile hexagon for Al-Ni-Co (left triple) and Al-Cu-Co (right triple). For each system, results with EAM potentials (left), ab-initio MD (middle), and pair potentials (right) are given.

Figure 3: Energy barriers of several diffusion processes with 3 atoms.

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D_{0x} [m^2/s]	6.5×10^{-8}	5.1×10^{-8}	1.8×10^{-7}	1.2×10^{-7}	1.8×10^{-8}	3.1×10^{-8}
D_{0z} [m^2/s]	3.5×10^{-8}	1.4×10^{-7}	6.3×10^{-8}	2.4×10^{-7}	1.6×10^{-8}	1.6×10^{-7}

Figure 1: Diffusion processes in the decagonal plane (Al-Ni-Co, Ni-rich). Dark grey, large: Ni; light grey, large: Co; dark grey, small: Al initial positions; light grey, small: Al positions after 100ps. Initial and final positions are connected. Dashed lines mark supertiles. Dotted circles mark three types of decagonal clusters, differing in the Ni content.

Figure 2: Atom density maps of a supertile hexagon for Al-Ni-Co (left triple) and Al-Cu-Co (right triple). For each system, results with EAM potentials (left), ab-initio MD (middle), and pair potentials (right) are given.

Figure 3: Energy barriers of several diffusion processes with 3 atoms.