Thermal diffusivity calculation.

Air:

$k = 0.024\ Wm^{-1}k^{-1}$
$C_p = 1005.0\ Jkg^{-1}k^{-1}$
$\rho = 1.225\ kgm^{-3}$

$\because \alpha = \frac{k}{\rho \cdot C_p}$

α = thermal diffusivity

k = thermal conductivity

C_p = specific heat

ρ = density

$\alpha = 1.9494\ m^2/sec \times 10^{-5}$

$\alpha = 1.9494 \times 10^{-3}\ \mathring{A}^2/as$

Water:

$k = 0.6089\ Wm^{-1}k^{-1}$
$C_p = 4196.0\ Jkg^{-1}k^{-1}$
$\rho = 997.0\ kgm^{-3}$

as - attosecond
Å - angstrom.

$\alpha = 1.4555 \times 10^{-7} m^2/sec$

$\alpha = 1.4555 \times 10^{-5}\ \mathring{A}^2/as$

$\because$ The simulation $dx = 1\mathring{A}$
thus the α value is converted to Å value

① Au - Gold:

[Nanomaterials]

$k = 314.0 Wm^{-1}k^{-1}$
$C_p = 129.0\ Jkg^{-1}k^{-1}$
$\rho = 19300.0\ kgm^{-3}$

$\alpha = 1.26 \times 10^{-4}\ m^2/sec$

$\alpha = 1.26 \times 10^{-2}\ \mathring{A}^2/as$