

Reverse NH₃ concentration effect on NH₃ induced hydrogen embrittlement

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Background and Objective



Potential hydrogen carrier
Carbon-free fuel

Important role in
Carbon Neutral Society

Objective:
Investigate the effect of NH₃ on HE

Take-out point:

We found **opposite** effect of NH₃ concentration on HE severity.

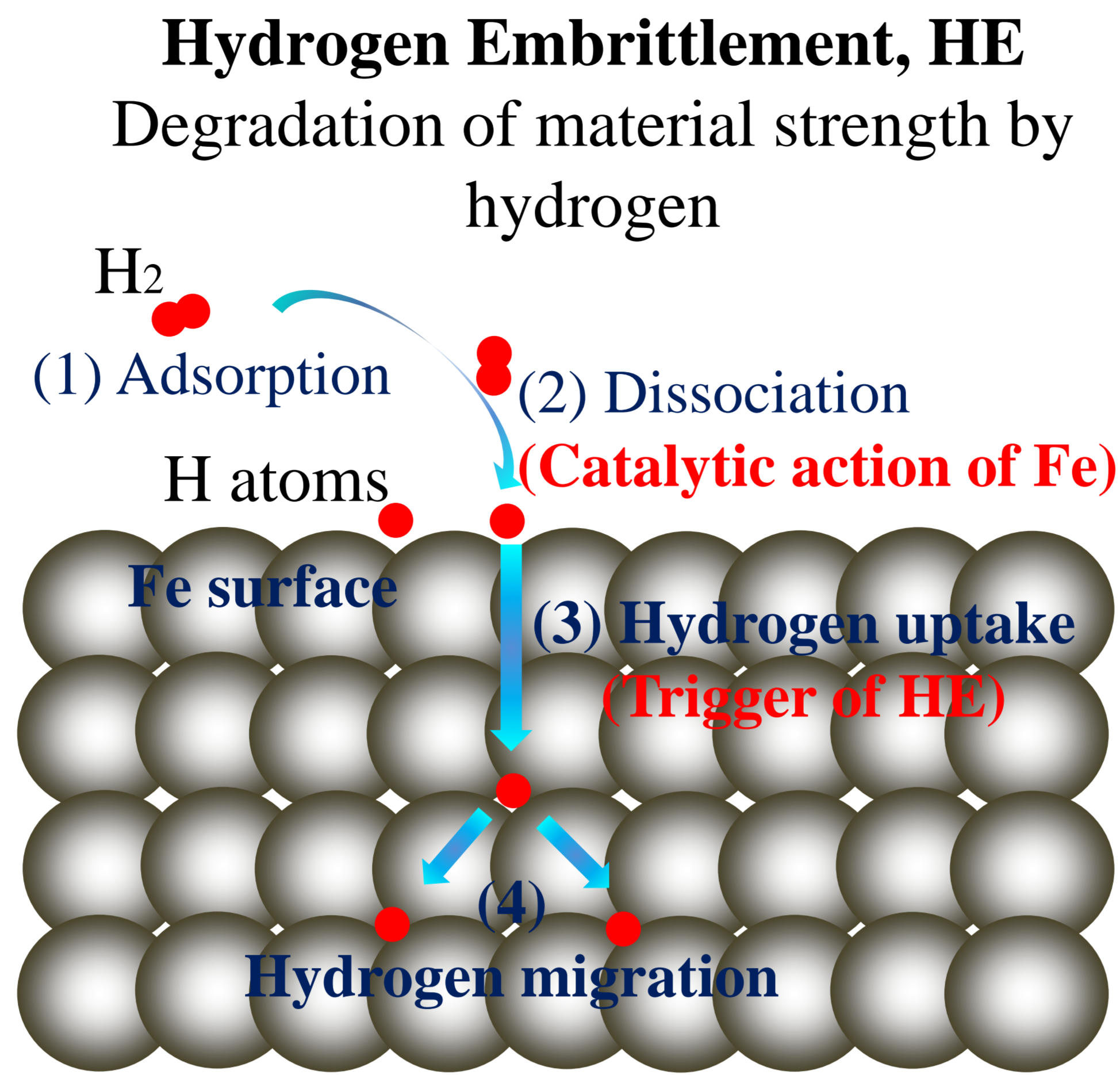
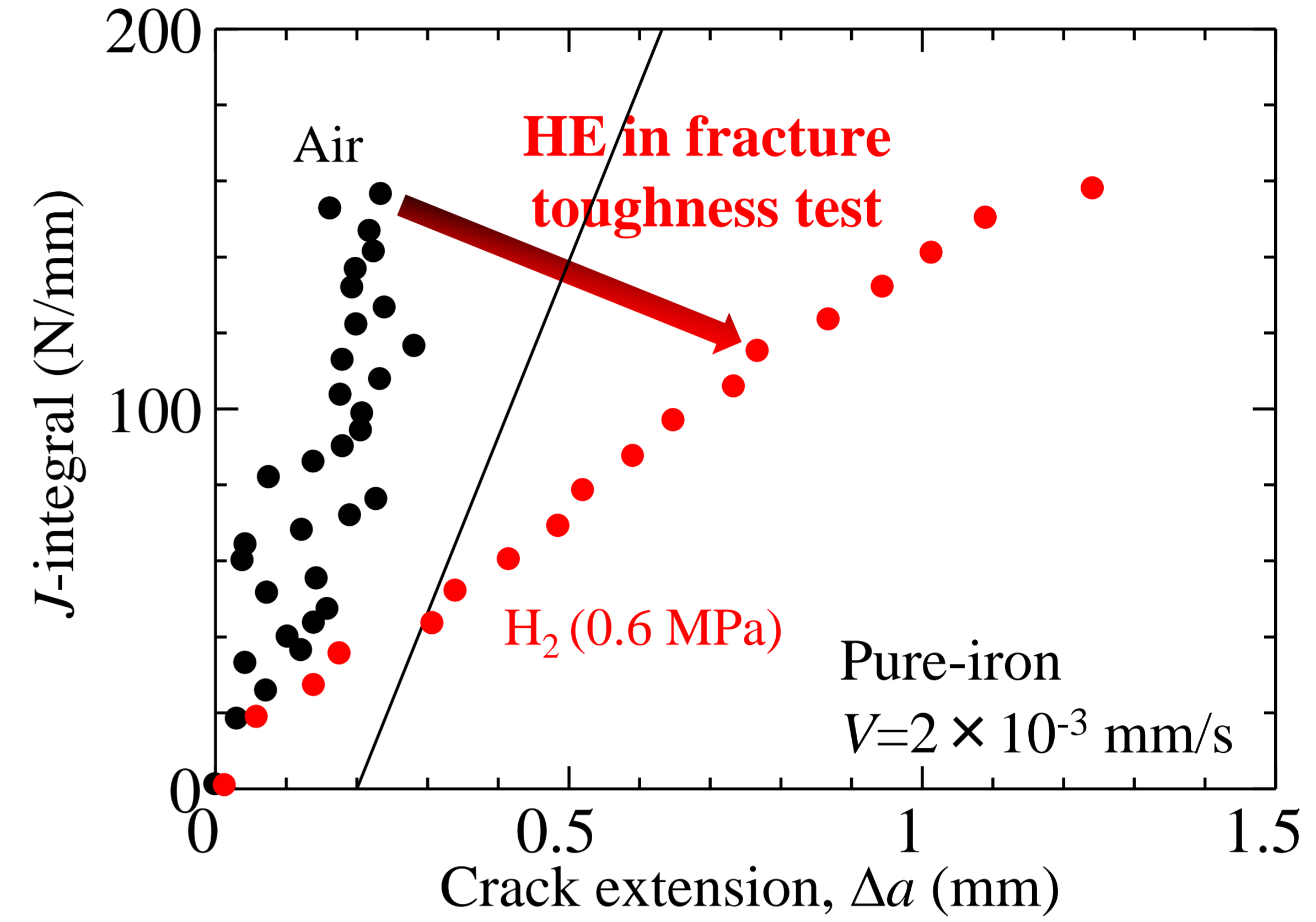


Fig.1 Hydrogen embrittlement in gaseous hydrogen

Degradation of fracture toughness by HE



A. Staykov et al, J. Phys. Chem, C 2019, 123, 30265-30273.

Fig.2 Fracture toughness test of pure iron

Fracture toughness test (J_{IC} test)

ASTM E 1820 standard

- Crosshead speed (V) : 2.0 × 10⁻⁵ mm/s
- Gas temperature : 293 K (room temperature)
- Gas pressure (p) : 0.1MPa
- Material : SCM440 (HV329)

- Gas environment
- High-purity N₂
- High-purity H₂
- N₂ + 1,000 vppm NH₃
- N₂ + 10,000 vppm NH₃

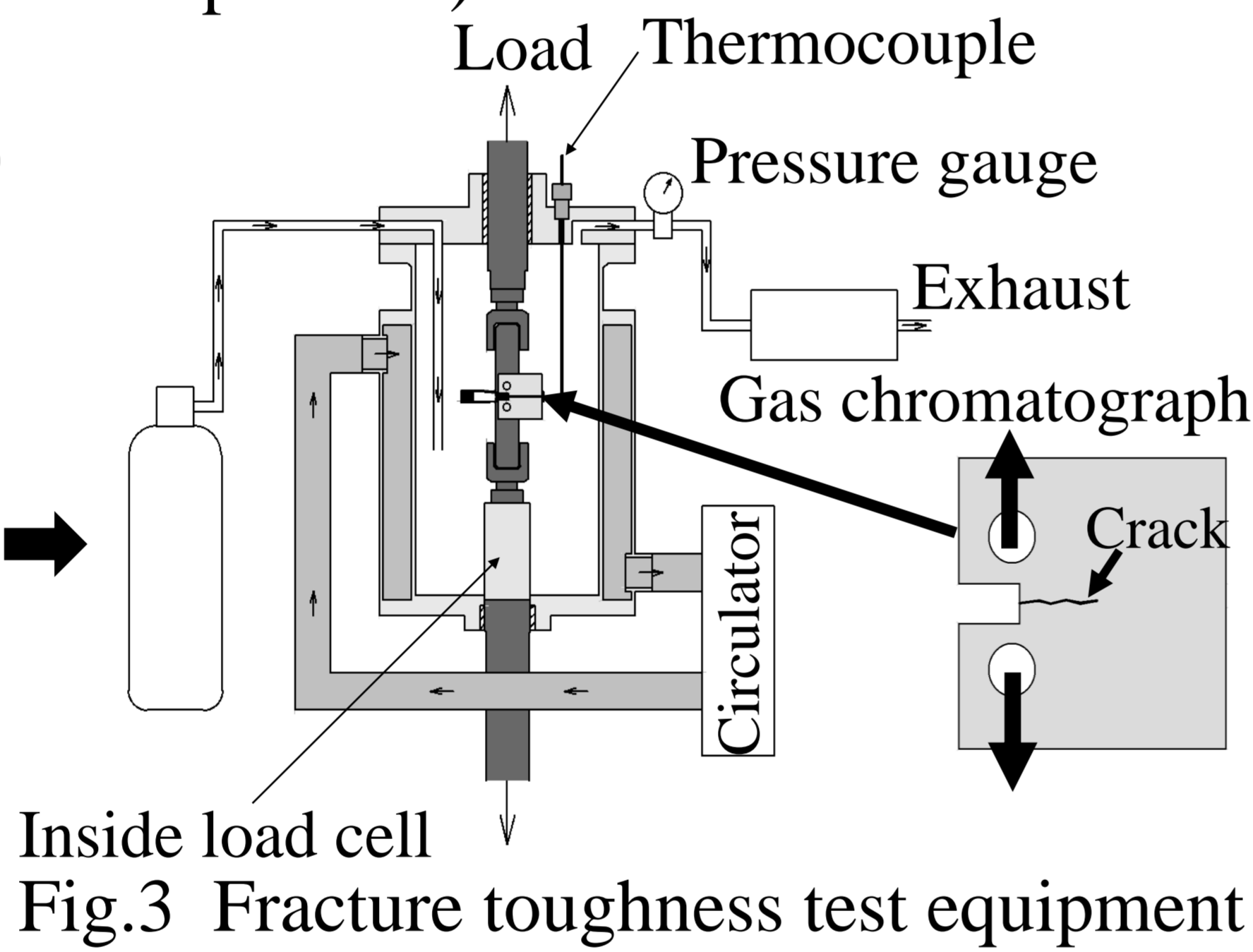


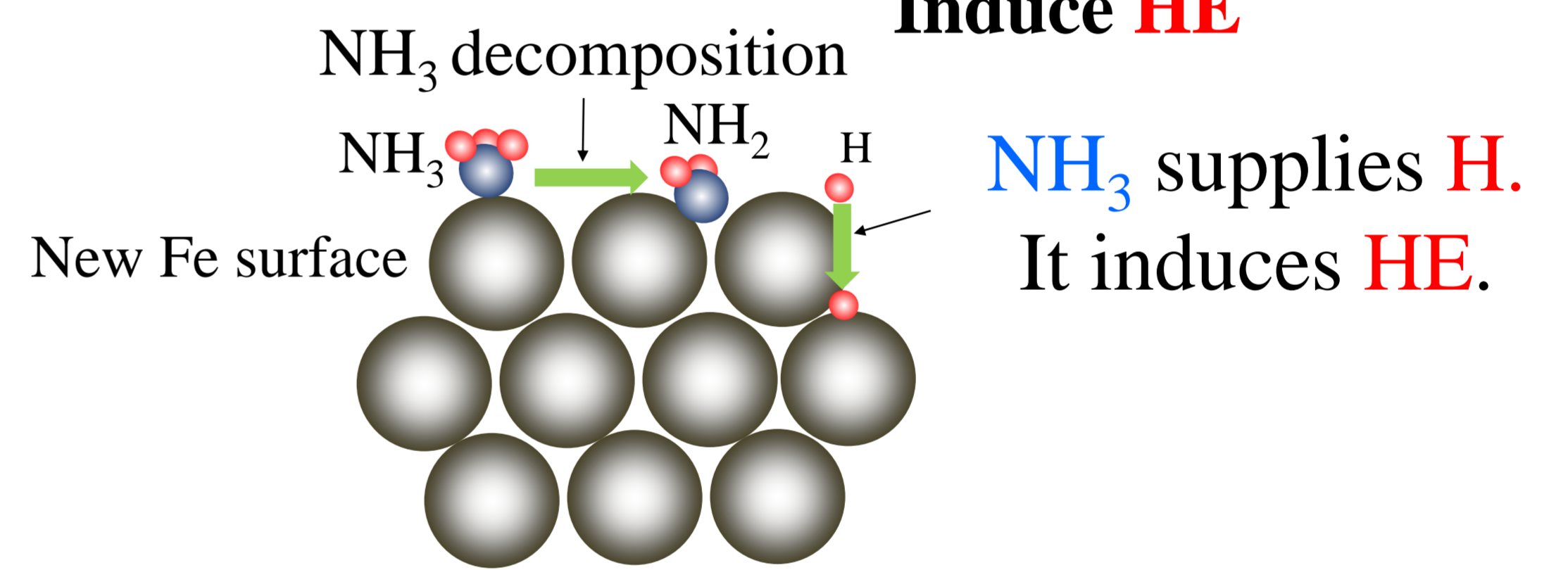
Fig.3 Fracture toughness test equipment

Discussion

Mechanisms of NH₃ induced HE



Induce HE



NH₃ is a source of H atoms by its decomposition

Effect of NH₃ concentration

NH₃ decomposition:

- (1) NH₃ → H + NH₂
- (2) NH₂ → H + NH
- (3) NH → H + N

For NH₃ adsorption, 1 site
For NH₃ decomposition, more sites are needed

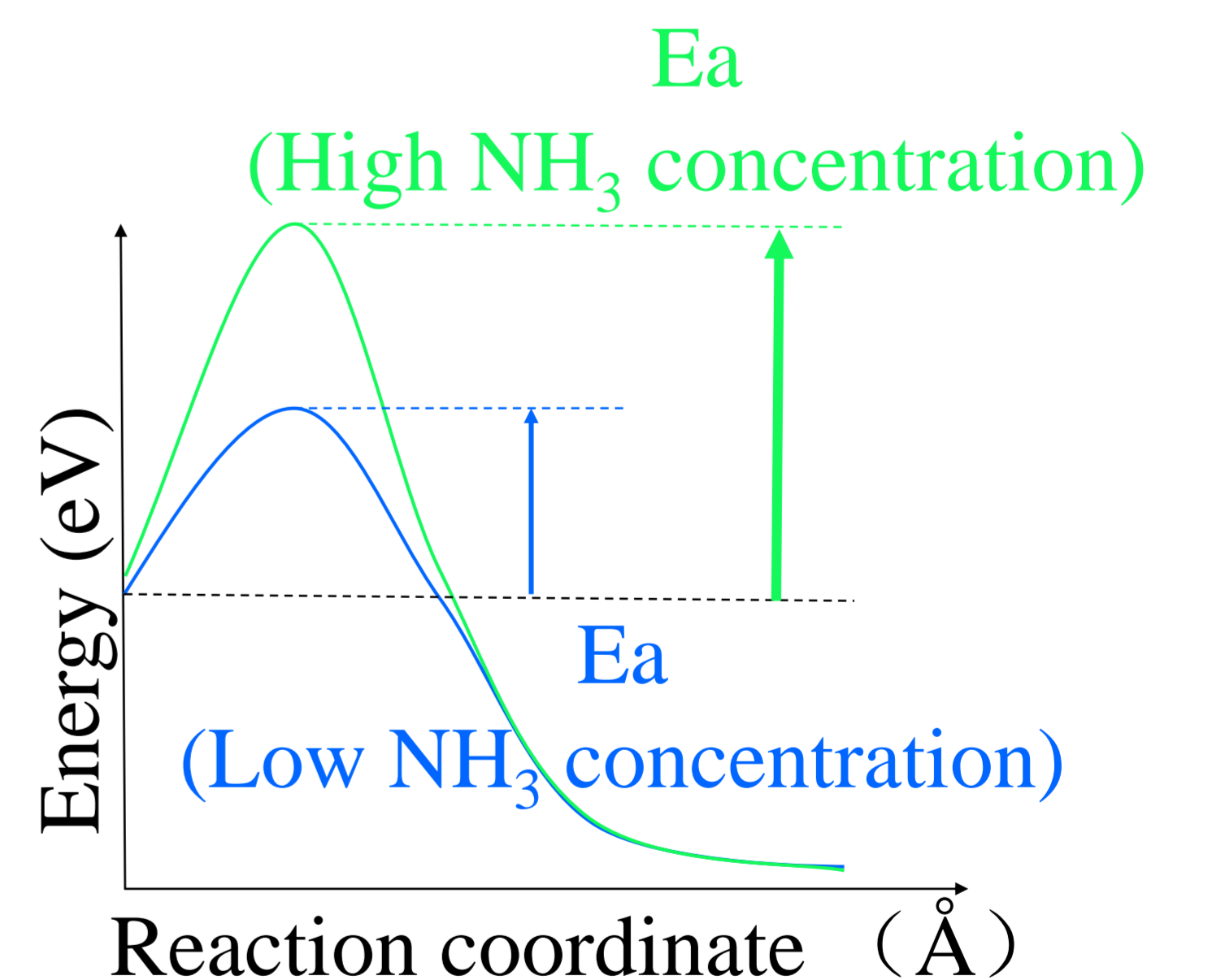
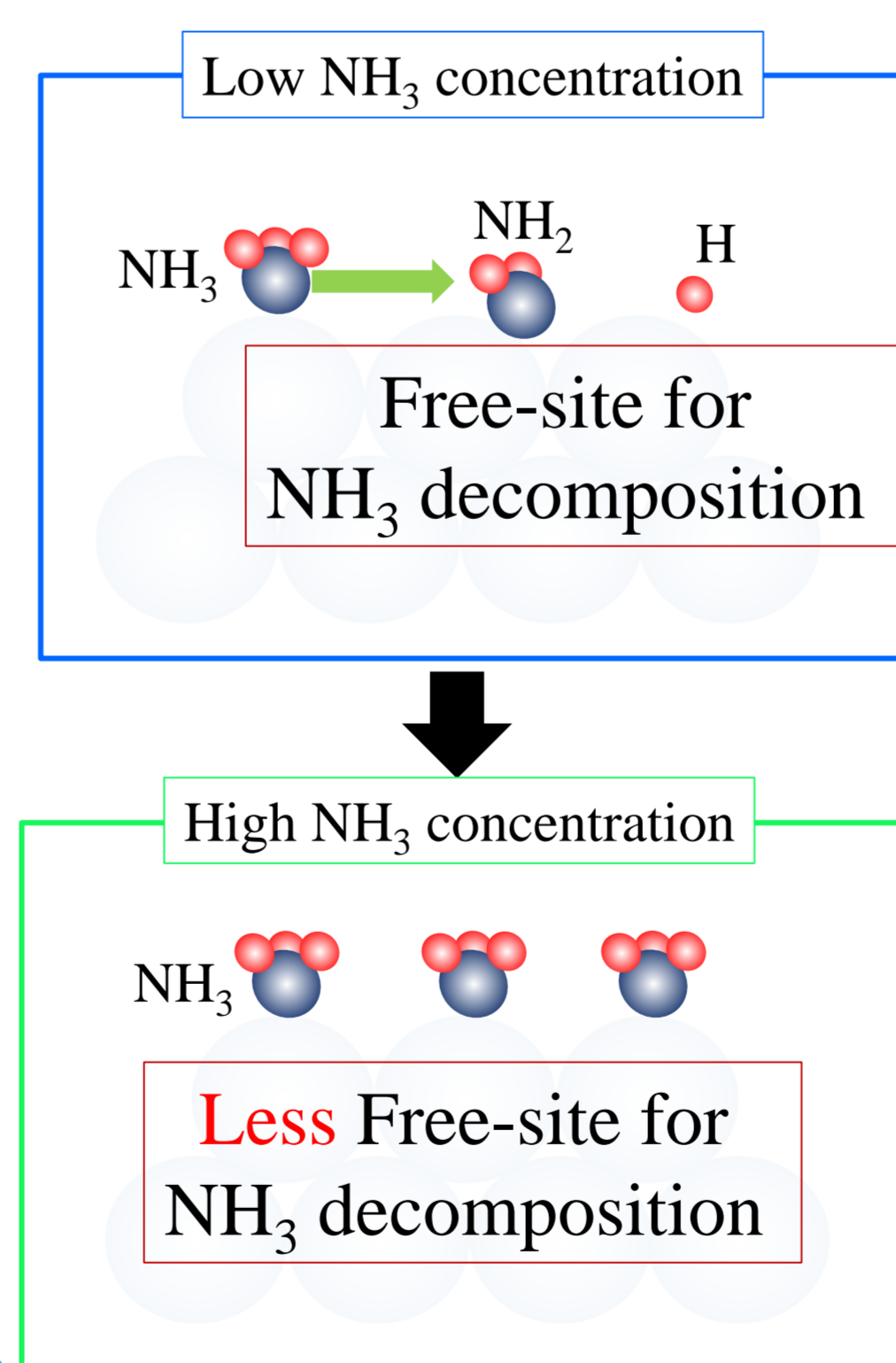


Fig.6 Ea of NH₃ decomposition (Ea: activation energy barrier of NH₃ decomposition)

Result

NH₃ can be the hydrogen source and can induce HE

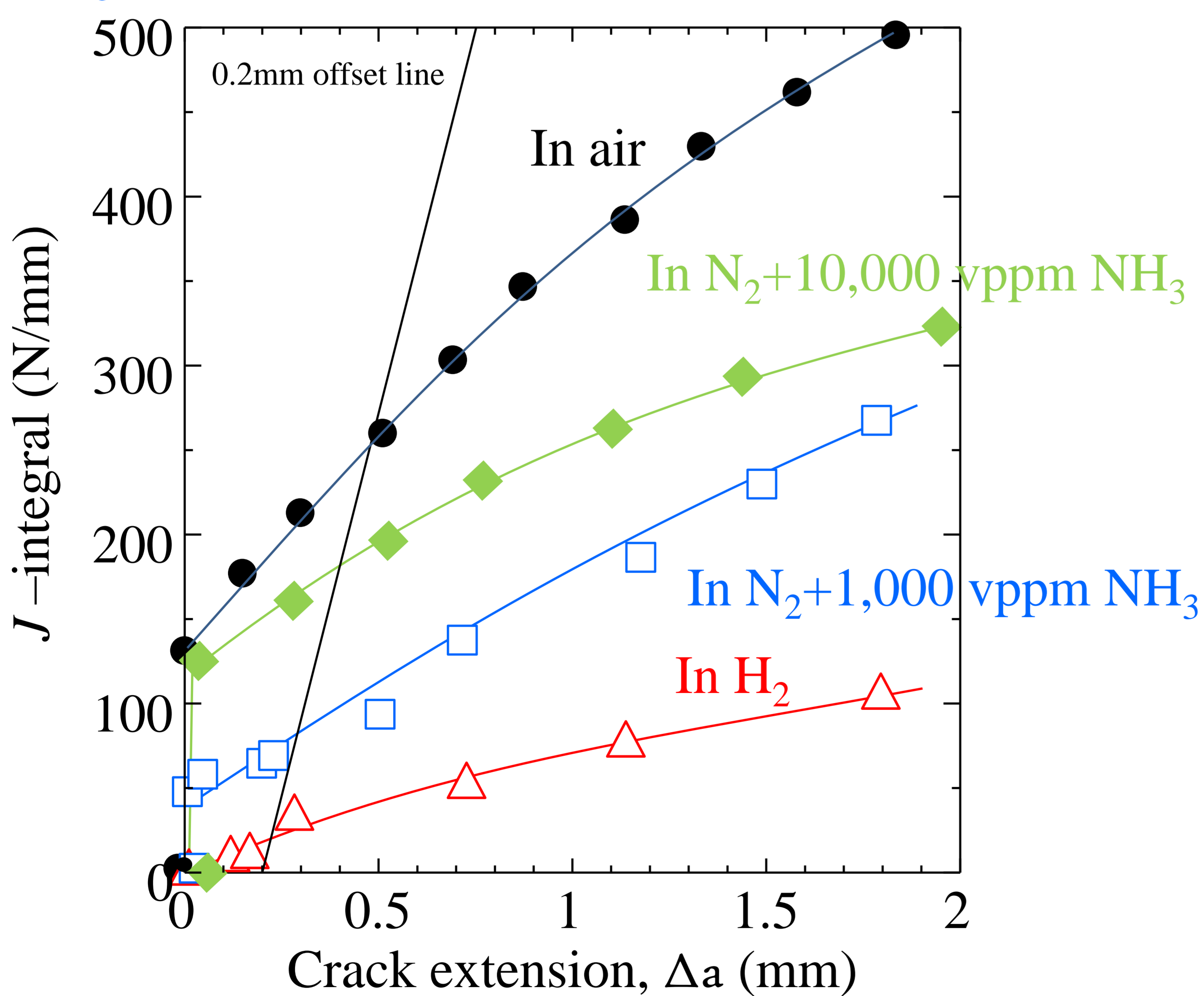


Fig.4 Fracture toughness test of SCM440

Prediction: HE became severer with increase in NH₃ concentration.
Result: HE with 10,000 vppm was less than that with 1,000 vppm.

Conclusions

The HE became less severe with the increase in the NH₃ concentration at 2.0 × 10⁻⁵ mm/s.

Mechanism of reverse NH₃ concentration effect

Increase NH₃ concentration

Activation energy of NH₃ decomposition increased

NH₃ decomposition became harder

Future Plan

Calculate NH₃ decomposition activation energy by DFT.