Niobium (Nb)

Chemistry, compounds and applications

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Element

Introduction[1]

- **1801; English chemist Charles Hatchett**
  - Atomic # 41 - ore sample from Connecticut
  - Initially called columbium (Cb)
- **Pegmatite in the form of:**
  - Columbite ($FeNb_2O_6$)
  - Tantalite ($FeTa_2O_6$)
  - Pyrochlore
- **Isotope niobium-93.**
- **1844; German Chemist Heinrich Rose noticed tantalum and other element called niobium**
- **1950; IUPAC adopted Niobium as the official name**

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[2]

Main Properties[1]

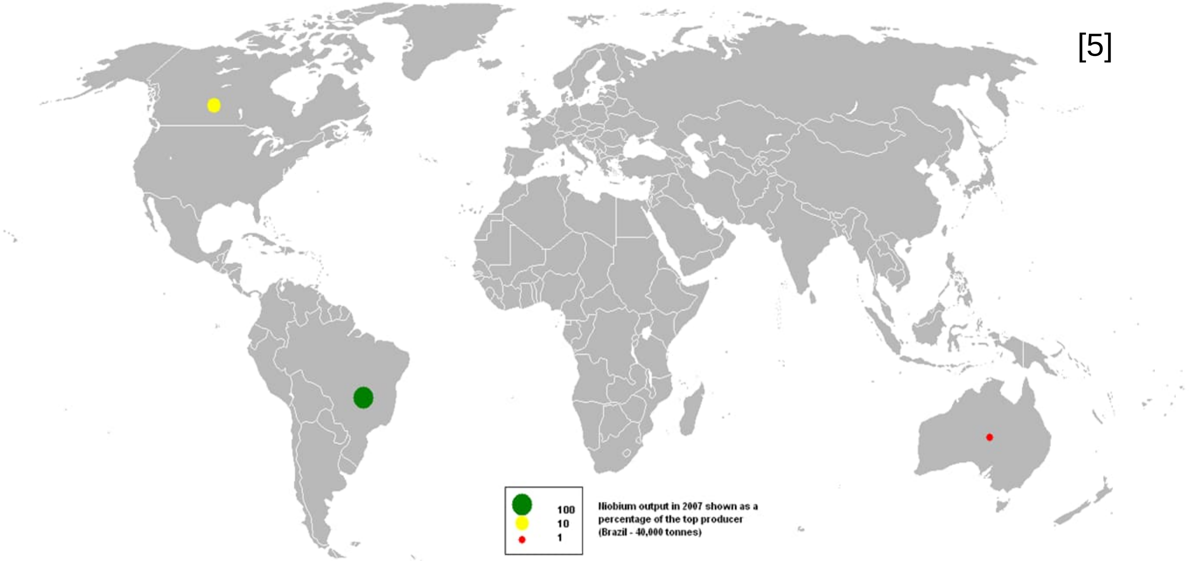
- **Transition Metal (M.P 2,477 C°)**
- **Soft and ductile**
- **Corrosion resistant**
    - susceptible to oxidation above about 400° C
- **Good ductility at room temp.**
- **Gray color**
- **Completely miscible in iron (ferroniobium)**

[3]

Availability & Demand[1]

- **Brazil (98.53%), Canada (1.01%) and Australia (0.46%) - Nb Reserves**
  - Reservations measures Brazilian niobium (Nb2O5) totaled 842.4 million tons, with an average grade of 0.73% Nb2O5

- **Brazil stand out with 98.53% of the world Nb mineable reserves, and is the largest producer of the metal, representing approximately 97.2% of the global total.**
- **Niobium is roughly 10 times more abundant in the crust of the Earth than tantalum**
- **Niobium, more plentiful than lead and less abundant than copper in the Earth's crust**



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Chemistry of Niobium

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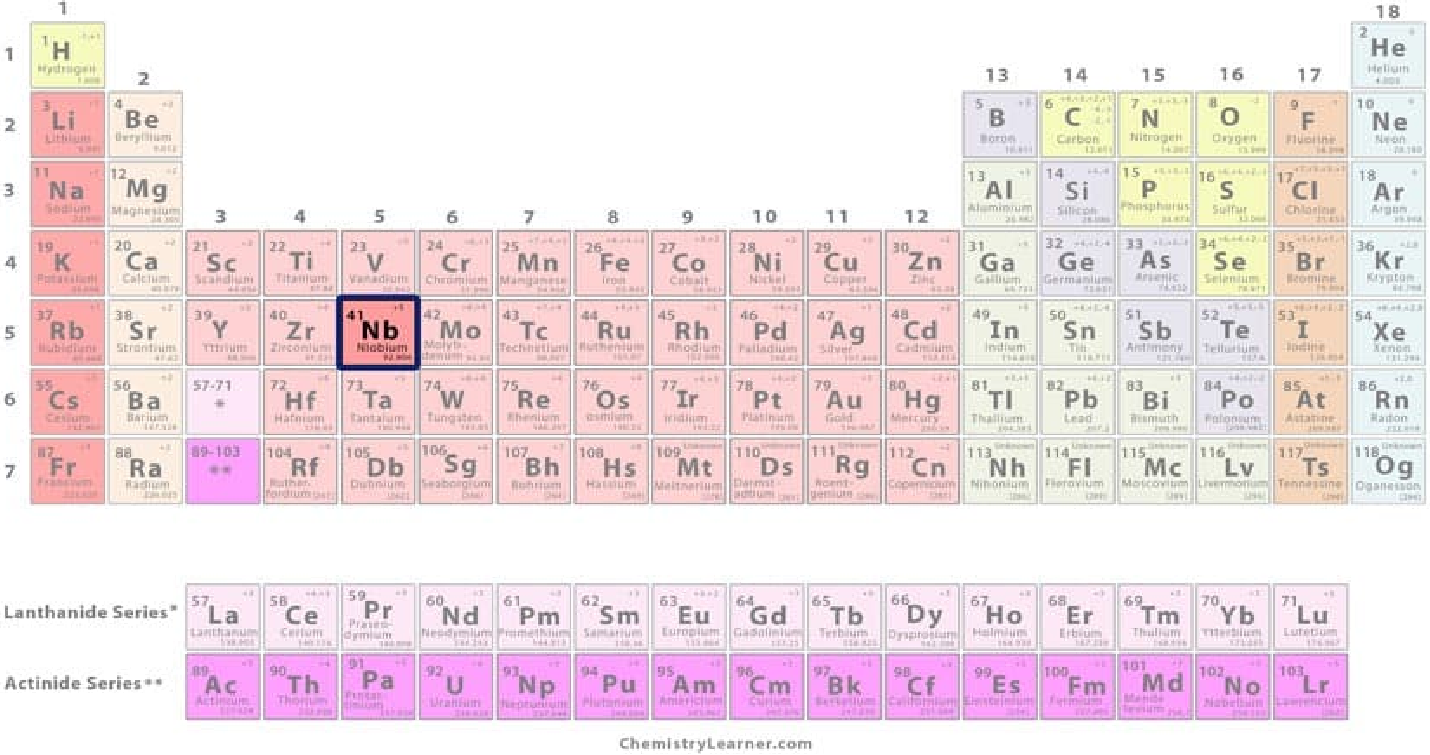
Location of Niobium in the Periodic Table



[14]

Niobium (Nb)

- 5d transition metal (four 5d-electrons)
- Most favorable oxidation state +V
- In RTS, Nb is very inert with hydrogen, air, water or acids (excl. HF and its mixture of HNO_3)
  - → When T is increased, Nb reacts with most non-metals and generates non-stoichiometric products [1]
- Only 1 stable isotope with natural abundance of 100%
- Similar chemical properties with tantalum

Chemical and physical properties of Nb	
Atomic number	41
Group	5
Period	5
Block	d
Electronic configuration	[Kr]$5s^1 4d^4$
Relative atomic mass	92.906 Da
Isotopes	1 (^{93}Nb)
Oxidation states	+V, (+III)
Atomic radius (van der Waals)	2.07 Å
Ionic radius (when oxidation state is +V)	0.64 Å
Ionization energy	652.13 kJ mol^{-1}
Crystal structure	cubic (bcc)
Lattice constant	3.3004^3 Å
State at 20 °C	solid
Melting point	2477 °C (2750 K)
Boiling point	4741 °C (5014 K)
Density	8.57 g cm^{-3}

[14, 16, 17]

Similarities between niobium and tantalum

- Tantalum (Z=73) is at the same group 5 with niobium.
- Both are d-block transition metals (Nb has 4 d-electrons and Ta has 3 d-electrons) and are solid in RTS.
- Their atomic sizes are similar (Nb 2.07 Å, Ta 2.22 Å) and both have a body-centred cubic crystal structure (a=b=c, α=β=γ=90°).
- Tantalum also has an oxidation state of +V (bond-forming with two 6s- and three 5d-electrons).
- Although similar with many chemical properties, tantalum is much denser (16.4 g cm^{-3}) with an atomic mass of 180.948 Da.
- Bigger size of Ta also increases the m.p. and b.p. of the element.

[17, 18, 19, 20]

Nb compounds and properties

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Compounds and their properties

Nb compounds can be divided: Niobium Oxides, Niobium Phosphates

Molecular Sieves Containing Niobium (e.g., Zeolites NbNaY) [16]

Group 5 metal exhibits compounds in oxidation states +2 to +5 [7]

Examples

- NbP: dark grey crystal and insoluble in water, exhibit extremely large magnetoresistance which can be used in electric components [5]
- NbB2: grey powder with melting point at 3050C -> ultra high temperature ceramic [6]

Metal Cluster Halides

- These highly symmetric clusters consist of a central octahedron constituted by 6 heavy metal atoms, stabilised by 12 bridging halogen atoms [8].
- 6 different cationic cores $\{Nb_6F_{12}\}^n$ $\{Nb_6Cl_{12}\}^n$ $\{Nb_6Br_{12}\}^n$

  $\{Nb_6I_{12}\}$ clusters remain yet to be synthesised. [8]
- The cluster is **remarkably stable** and can undergo oxidative addition to form $[M_6X_{18}]^{2-}$ clusters, in which one halogen atom has attached terminally to each metal atom [7]
- Require significant development with possible applications in catalysis and bio–medicine [8].

CHAPTER 21 • Properties of the 4*d* and 5*d* Transition Metals

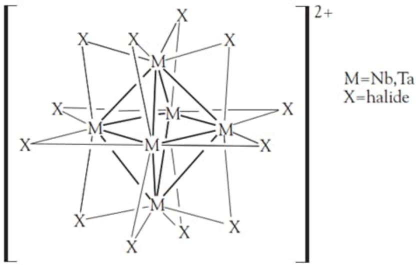


FIGURE 21.8 Structure of the $[M_6X_{12}]^{2+}$ ion, where M = Nb or Ta and X = halide.

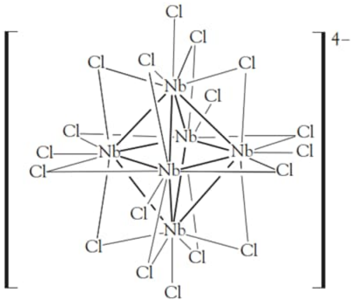


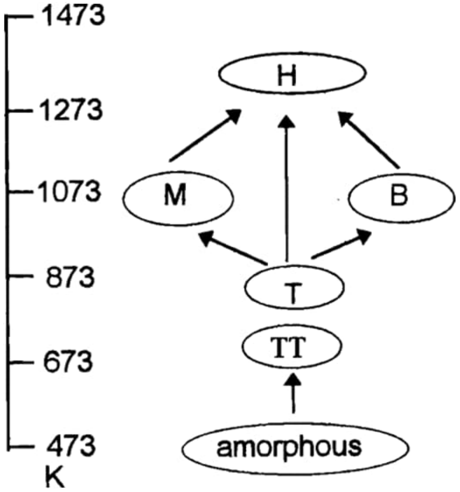
FIGURE 21.9 Structure of the $[M_6X_{18}]^{2-}$ ion, where M = Nb or Ta and X = a halogen.

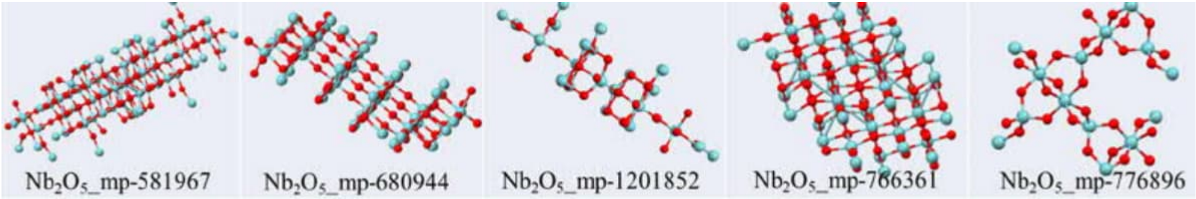
Nb_2O_5

- Niobium pentoxide is a white, air-stable, water-insoluble solid.[8]
- **Production**

$$2\ NbCl_5 + 5\ H_2O \rightarrow Nb_2O_5 + 10\ HCl$$

- **Nb_2O_5** possesses a quite complex crystalline morphology and about 20 different structures have been identified





[10]

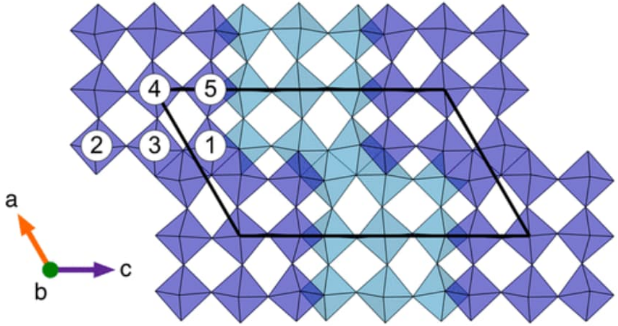
Applications [1]

Table 3. Some types of products Nb and applications[12-20].

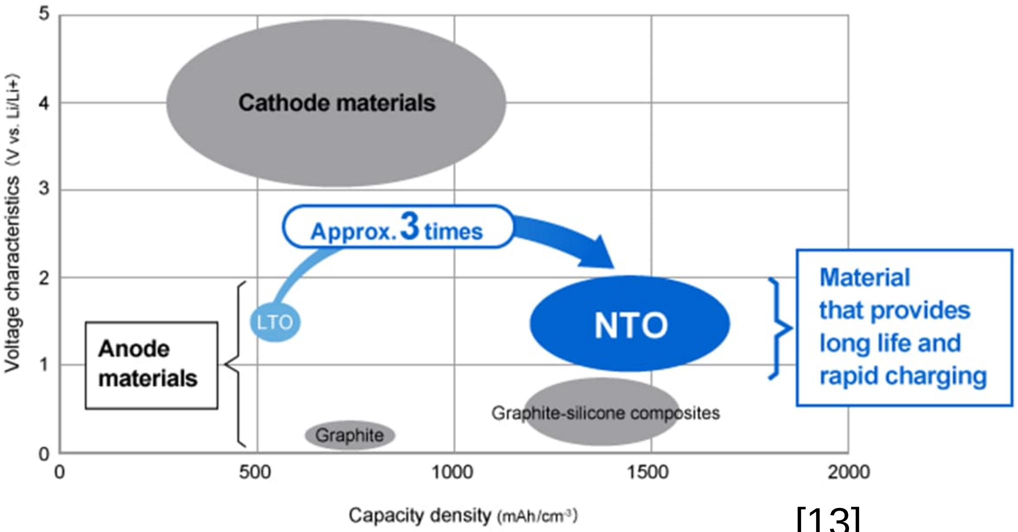
Niobium Species	Principal Properties	Applications
Nb oxide	High index of refraction High dielectric constant Increase light transmittance	Camera lenses Coating on glass for computer screens Ceramic capacitors Manufacture of lithium niobate for surface acoustic wave filters
Nb carbide	High temperature deformation and controls grain growth	Cutting tool compositions
Nb powder	High dielectric constant, stability of oxide dielectric	Nb capacitors for electronic circuits
Nb metal	Corrosion resistance	Chemical processing Equipment
FeNb	Weight reduction, increased strength and toughness due to grain refining	Nb additive to high strength low alloy steel and stainless steel
Nb titanium and Nb tin alloys	Very low electrical resistance of alloywire at low temperatures	Superconducting magnetic coils in magnetic resonance imagery

Titanium Niobium Oxide – Fast charging battery [22]

- $TiNb_2O_7$ is being developed as a high-energy-density alternative anode material to $Li_4Ti_5O_{12}$ for specific market sectors
- The reaction of $TiNb_2O_7$ with lithium is not as well-defined
- The reduction to $Li_3Ti^{III}Nb^{IV}{}_2O_7$ (one lithium per transition metal) occurs at ~1.4 V vs Li^+/Li, providing a theoretical capacity **of 232.6** mAh g^{-1}.
- The reaction proceeds further as the voltage is decreased and can proceed to $Li_5Ti^{III}Nb^{III}{}_2O_7$ with a theoretical capacity of **387.7** mAh g^{-1}.



Titanium Niobium Oxide – Fast charging battery



[13]

TOSHIBA

Application Of Niobium In Alloy Steel[11]

- **Increase strength, mechanical, welding properties and corrosive resistance**
- **Low-alloy high-strength steel (80% Nb)**
  - small amount of niobium to form stable carbides and carbonitrides
  - precipitation of niobium carbide can improve the strength and creep resistance of the steel.
- **High-alloy steels**
  - additives metal niobium bars or ferroniobium (50-70% Nb)
  - stainless steel, heat-resistant steel, and corrosion-resistant steel

Application Of Niobium In Alloy Steel[11]


[12]

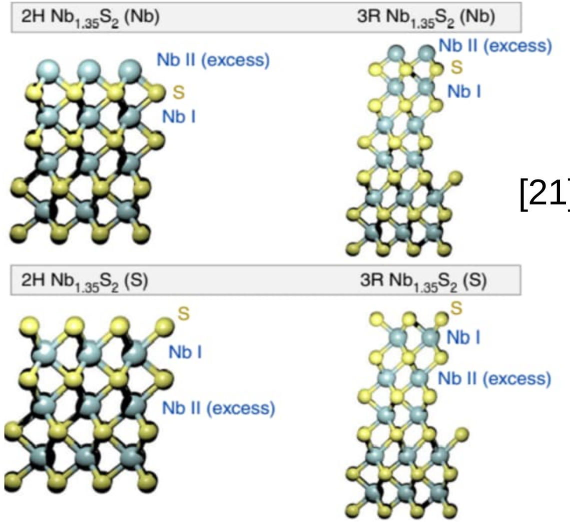
- **Niobium has showed improvements in the production process**
    - melt shop, Niobium result in less oxidation, where the efficiency of FeNb is about 95%,
    - FeTi ranges from 80 to 85%.
- **Niobium also avoid clogging during casting**
- **Considerable effect on the pitting corrosion**
    - increase of Nb content in the matrix which causes “beneficial disorders” increasing corrosion resistance by the formation of Niobium Oxides
    - higher protection than Chromium oxides

Niobium disulfide NbS_2 could be a viable catalyst for the hydrogen evolution reaction (HER)

- Transition metal dichalcogenides (TMDs) are good catalysts for the hydrogen evolution reaction
- However, noble metals like Pt have a current density of >1000 mA/cm^2, while TMDs such as semi-conductive MoS_2 have a current density of ~10-100 mA/cm^2
- Lower current density for many TMDs is caused by proton-adsorption on their surface in the first step of HER, decreasing the conductivity of 2D nanosheets

[21]

An electrolyser based 2H $Nb_{1+x}S_2$ cathode can generate current densities of >1000 mA/cm²



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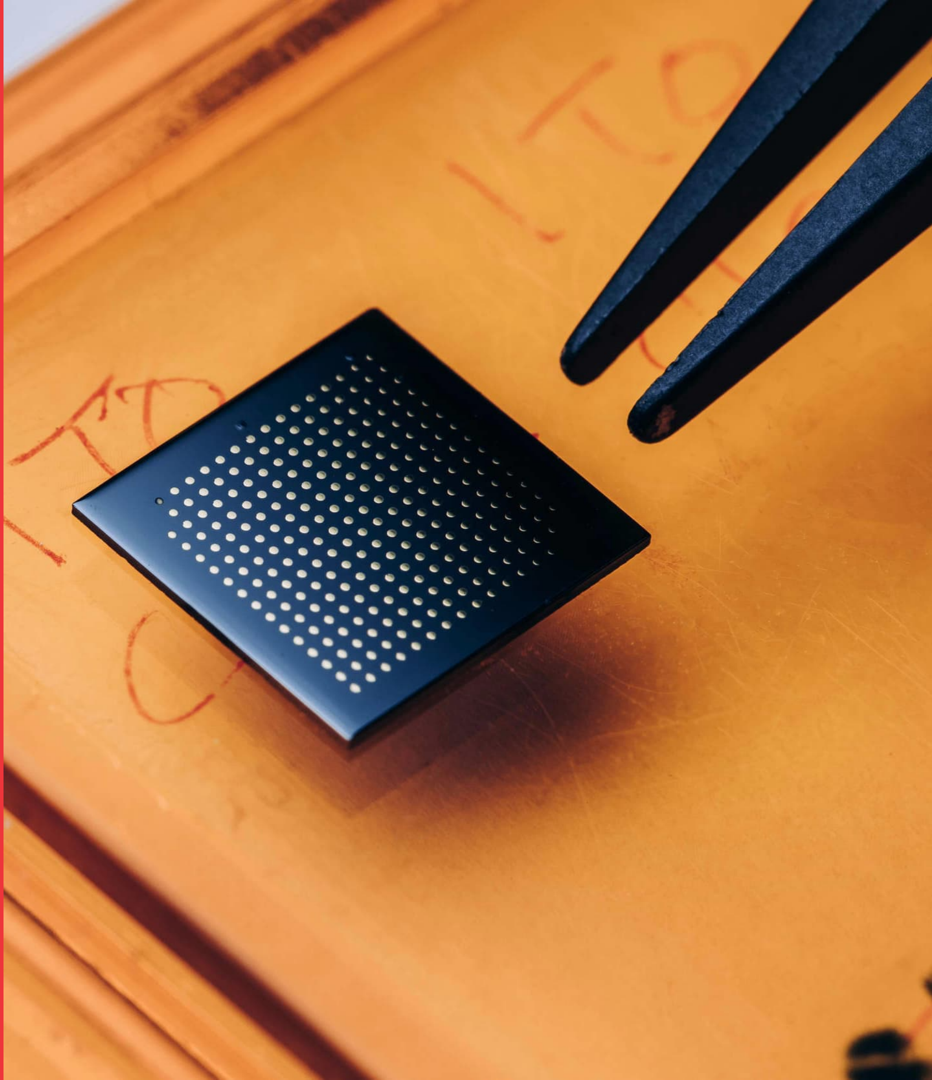
- Layered 2H (hexagonal) NbS_2 is predicted to be one of the most efficient TMD electrocatalysts for the hydrogen evolution reaction
- Metallic 2H $Nb_{1+x}S_2$ (where x ~ 0.35) with additive niobium does not have the van der Waals gaps between its layers, so the conductivity improves → reaching up to same current densities than with Pt or Ir

[21]

Questions?



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